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Dedicated to Jans, Yvonne and Harald, Bart and Petra, and my grandchildren Sanne and Eva

"Imagination is more important than knowledge"

Albert Einstein

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Foreword

The very rapid development of the chemical industry after the Second World War has been accompanied by an equally rapid development of the science of chemical engineering. Simultaneous developments in other engineering disciplines have enabled the manufacture of new and much better equipment and instrumentation for process plants. During the 1970s, a high level of efficiency was reached, so much so that even now some researchers in the field insist that it was during that decade that process design discipline reached maturity. However, new demands by the public have led to an increasing amount of attention being paid to aspects of safety and environmental protection. Moreover, progress in the fields of mathematics, informatics, physics, and electronics have major implications for chemical engineers. Today, most design methods for equipment have been converted into software so that many routine tasks can be carried out using a computer.

During recent years, an awareness of the limited availability of raw materials and energy sources, together with the high priority for environmental protection, have led to an intensification of the interaction between different relevant disciplines. In addition, the globalization of chemical enterprises – leading to larger sizes of chemical companies and a much stronger competition world-wide – demands much more awareness of the strengths and weaknesses of a company's own specialists compared with that of their competitors. Competition demands strict control of investments. Companies will build their plants wherever the best economics are achieved, and hence investment in plants will be carefully controlled. Whilst savings on investments implies that more plants can be built with the same available funds, even greater new demands will have to be met in the 21st century! Technology will be judged on the basis of its sustainability, and in the future new renewable raw materials will have to be used for our daily goods, energy, and fuels. Moreover, processes will need to become an order of magnitude more reliable.

Over the years, many scientists have pondered the fundamentals of engineering disciplines, including the strategy of process engineering and the logistics of chemical manufacturing. In turn, this has led to many system studies and even schools of study of the process design engineer's work. Although many rules and regulations have been developed for system studies, production scheduling and production logistics, very few of these are actually used in the process industry. Much can be learned from positive achievements in the mass production of consumer goods. Indeed, we may ask ourselves whether the chemical engineer has reached the same level of maturity as the manufacturers of consumer goods.

It is to the great merit of Jan Koolen – a process design engineer of many decades experience – that he reflected long term about the essential tasks of a process design engineer. With regard to other products, Jan feels that even the design and production of a relatively simple unit such as a freezer is a challenging example for chemical plant designers – and a great incentive for them to create improvements. Such a machine may run unattended for 15 years, and with very simple control – especially when compared for example with the cold sections of cracking plants for olefins! In this regard, Jan's vision is that we must move towards the use of robust and simple plants. He is a pioneer in this field, and this book proves that there is still much scope for improvement by the designers of process plants. Jan's faculties of abstraction, combined with his long-term experience in process design, have resulted in this first practical book on robust and simple design, covering the entire field of chemical engineering. This book will prove to be an indispensable tool for all engineers in the operation, design, and development of processes. Moreover, it will inspire them in their daily work, and also open their eyes to the many opportunities and challenges that they will encounter in the future. Highly experienced process designers will also find stimulating suggestions in this book, and we can be sure that it will have a major impact on our future plants, making them – in time – better, simpler, and more robust!

The Netherlands *K. Roel Westerterp*

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Preface

My experiences in the process industry during the past decade led me to write a book about the design of simple and robust process plants which include reliable, hands-off operation. There was, I felt, a clear short-coming in that nobody had published a comprehensive work covering this subject – a somewhat surprising finding since the benefits of such a designed process are huge, with capital savings on the order of 30–40% achievable compared with a conventionally designed process. Moreover, operational savings can also be achieved by minimizing operational personnel and improving the quality of operation. A limited number of reports have been made on process intensification which address the concept from a unit perspective. The present book tries to create a total picture of how the design of a truly competitive process should be approached, from process design through control design to operation.

One question which I have to answer quite often is, "Why do you think *now* is the right time to introduce this concept"? The answer must lie in the progress that has been made in technology:

- The mechanical design of equipment has been improved by better design details. Of special mention here is the drive to minimize or eliminate mechanical contact, for example the introduction of gas seals first for compressors, and currently for pumps. Screw compressors have been introduced with synchronized, separate electric drives for both screws in order to avoid metal-to-metal contact of the gears. Another example of avoiding mechanical contact is in switch design, these being changed from mechanical to inductive types. Next to other mechanical improvements, these designs have been improved over the years, and resulted in more reliable components with longer stand times so that maintenance could be minimized and times between shut-down for mechanical reasons increased. This is one reason why the philosophy "Design for single components unless ..." is introduced.
- Process technology has improved by means of simplification and intensification. During the past few decades, progress has been made to minimize equipment, improved logistic operations have been applied, storage has been reduced, and the quality operation has been improved to avoid off-spec facilities. In addition, several functions have been combined into one vessel, for

example reactive separations or divided wall column distillation for three-component distillation, and equipment has also been combined. Process intensification efforts lead to a reduction in the size of equipment by increasing the surface area per volume, increasing transfer coefficients by turbulence generation, and utilizing centrifugal forces ('highgee') to achieve improved phase separation. The process and control technologies have also benefited from the enlarged capability of modeling the processes, both statically and dynamically.

- Computer technology has made tremendous progress, and this has enabled the development of digital instrumentation systems with powered processors where models can be used to enhance control processes. Computer technology also permits the dynamic modeling of process plants that makes the design of control a reality, while optimization optimizations models can be applied with reasonable response times. The application of integrated circuits (ICs) for smart instruments is a spin-off which makes instruments more accurate and reliable, while communication technology has been so greatly enhanced that the remote operation of process facilities is clearly achievable.
- Operational and control design based on first-principle dynamic models is now a reality. The design of operational procedures to comply with first-pass prime production can be supported by dynamic models. In addition, control technology has been developed to a point where analyses based on dynamic models can be made available to judge design alternatives on controllability. The critical control loops can be tested and tuned in closed loops in simulations to support robust control.

This book has been written with students, engineers, and managers involved in the design and operation of process plants in mind, the intention being to provide them with an approach for the different design and operational aspects to design simple and robust process plants. The design techniques for sizing of equipment are not described, as there are many publications in this field. Although most examples are taken from the chemical industry, the approaches are similar for other processes such as food, pharmaceutical and water treatment plants.

Despite the vast amount of material that has been combined and structured into this book, a great deal of imagination and conviction will be required in order to achieve a design which deviates structurally from the well-trodden pathways of traditional design approaches. Put simply, this can be re-phrased as:

"The design of an optimal designed safe and reliable plant, operated hands-off at the most economical conditions becomes a reality".

The Netherlands *Jan Koolen*

For those who want to comment on the book or have valuable additional information about process simplification please feel free to contact me. E-mail address: ILA.KOOLEN@wxs.nl

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Acknowledgments

Writing a technical book requires not only a lot of reading, but also many discussions and extensive support from colleagues who are active in the field of interest. Without this support it would not be possible to prepare a work such as this. The discussions and support are not limited to the time during which the pre-work and writing is carried out, and most of the technological knowledge has been collected during the working years of my life, and from academic relationships. Therefore, it is virtually impossible to mention all those people who have in the past contributed to my personal knowledge and consequently made writing the book more fun than exercise. Hence, my first acknowledgement is to all these 'un-named' individuals.

The work could not have been prepared had I not received complete support from The Dow Chemical Company during preparation of the manuscript. There was, in addition to excellent office and library facilities, the even greater advantage of direct contact with engineers who were active in the field, and it was they who made me aware of recent developments of in the technology. The individuals to be mentioned who personally created this possibility at Dow are; Theo van Sint Fiet, Sam Smolik, and Doyle Haney.

In writing this book, perhaps the greatest encouragement came from Roel Westerterp, who stimulated me to write from an industrial insight – thus making it different from other volumes that mostly address specific design issues. It is my great pleasure that he agreed to write the foreword.

The individuals who supported my work with their knowledge and experience, and who gave their time for discussions and reviews of the manuscript are mentioned in order of the chapters.

Several chapters were reviewed by Paul van Ellemeet, who provided me with valuable comments on the style of the manuscript. In discussions on the simplicity of a process, what makes it complex, and what the term 'robust' means, Peter Wieringa was an excellent debating partner, and also provided me with excellent reference material. The design philosophies were reviewed by Jan Willem Verwijs, who also gave valuable suggestions on how to promote the messages, while process synthesis and simplification were extensively reviewed by Henk van de Berg, who was my sparring partner in this field.

With regard to process integration, the help of Stef Luijten and Guy de Wispelaere was of great value, and reliability engineering was the area where the knowledge and experience of Rudi Dauwe is greatly reflected. Indeed, without his help these chapters would not have been included. The text on instrumentation was provided largely by Cees Kayser and Rob Kieboom, while for operation automation Herman Liedenbaum was my reference partner. Of particular note regarding the implementation of transient operations of critical reactor systems and reactor control was the irreplaceable support from Jan Willem Verwijs. Hands-off control of process plants requires advanced control techniques and in its practical implementation the support of Raph Poppe was hugely encouraging. The search for self-optimizing control structures found its place in this book through my contacts with Sigurd Skogestad. Control strategy design based on first-principles dynamic modeling was more than supported by the Dutch control community, and specifically by John Krist, whose knowledge and experience regarding process optimization are reflected in the text. It were Mark Marinan and Ton Backx who gave me their insight in how to deal with operation optimization and its reflection to model based control. The methodology for implementation of value-improving practices during a project is based on the approach of IPA (Independent Project Analysis, Inc.), represented by Edward Merrow, and from whom full support was received.

The editorial work of Bill Down was highly appreciated, this certainly contributed to the style of the book

My appreciation goes to all those individuals who are (and also those who are not) mentioned and who contributed to my knowledge and understanding, and as such find their contribution reflected in the manuscript.

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Chapter 1
Introduction

This book covers the design of simple and robust processing plants, and is intended to inform managers and engineers in the process industry of the opportunities that exist for the development of much cheaper and improved designs. The application of the concept is not limited to the chemical industry, but rather covers the process industry in general. Potential savings that are achievable on capital are in the order of 30–40 %. The plant of the 21st century is defined as being the objective for a simple and robust processing plant, while the design philosophies, techniques and methodologies that might make this a reality are explained in detail. One of the reasons for simple design opportunities – next to conservatism in design – is the evolution of auto-complexification (Scuricini, 1988). The argument is that large technology systems are subject to an evolution, and that this results in more complex systems. Greater complexity is achieved by an increase in the number of components, procedures, rules and data handling. The opportunities to enhance the design of processes are numerous, and many examples will be used to illustrate potential improvements This book is not intended to inform the readers how to calculate the different design, although the necessary design principles and approaches to achieve simple and robust designs are outlined. In reading this book, engineers will appreciate that the concept requires a broad view on process design.

1.1
A New Evolutionary Step

The design of chemical plants experiences a new evolutionary step. During the past decades, a number of developments have been seen in the processing industry that are considered trend setting for future process plant designs. These include:

- Improved modeling and computational technology:
- – Capabilities for static and dynamic modeling and simulation have made great progress, being complemented with optimizers to achieve optimal designs and operations.
- – The development of pinch technology for streams that can be optimized and reused, such as energy, water, and hydrogen has also advanced.

- Capabilities for mixed integer design problems are within reach for commercial software. The modeling of flow dynamics is another area where progress has been made in the understanding and improvement of process design. In particular the introduction of reaction kinetics and multiphase behavior can be included in the computations.
- All these modeling capabilities are supported by a strongly increased computational power. With these modeling technologies it is easier to understand the process technology and so achieve improved designs and operation.

- The reliability of industrial components. This has also been improved considerably, with the mean time between failures (MTBF) of components having been increased over the years. This is reflected in the ongoing efforts of vendors to make their products more reliable. Plants often have in-house reliability engineers to perform root cause analysis of failures; based on these analyses, modifications are implemented to achieve higher plant reliability. The time between turnovers of process plants has increased to more than 4 years. In cases where systems are subject to process fouling or aging, the reduction of these problems receives similar attention in order to achieve longer operational uptimes.
- Higher automation levels and robust control. The introduction of process computers has resulted in automatic start, stop and regeneration procedures, with less variability and fewer operational errors. Improved instrument design, with the development of on-line analyzers and adequate control design, brings hands-off operation within reach. These improvements in communication technology has made remote monitoring and operation a reality.

These technical capabilities, the economical circumstances, and the environmental requirements have resulted in the development of more efficient processes with regard to raw material and energy utilization, together with greater compliance with more stringent environmental and safety requirements.

Table 1.1. Technical comparison between domestic and industrial refrigerators.

Technical point	***Domestic***	***Industrial***
Safety devices	–	17
Instruments to control system	1	58
Instruments, local	–	20
Control loops	1	9
Valves	–	120
Equipment*	2	10
Filters	–	5
Reliability	Very high	To be proven
MTBF (years)	>10	1
Spare unit	None	One

* As experienced by the operator.
MTBF = mean time between failures.

The above-mentioned technical developments may form the basis for improved plant design and operation, but much work still needs to be done. To illustrate this, the installation of a domestic refrigerator – an example of a *simple and robust design* – is compared with an industrial refrigerator with an installed spare unit. A comparative list of devices contained in both units is shown in Table 1.1.

This example shows that a reliable unit can be built, but it also shows that there is a vast difference in the design of a domestic unit and that of an industrial unit (Figures 1.1 and 1.2). It is also obvious that domestic refrigeration units went in the direction of robust design, due to customer requirements. Next to the reliability of the unit, customers also require competitive investment, low operational cost and simple operation with no maintenance. Thus, the domestic refrigerator as a simple and robust design is an ultimate example of:

An optimal designed safe and reliable unit, operated hands-off.

The meaning of simple and robust designs will be discussed in **Chapter 2**. As an example, it will be explained why a piping manifold – which in essence is a simple piece of equipment – can be complex to operate (often, we have many line-up possibilities, where operators have much freedom), although such a system is not error-tolerant. This can be compared with a television set, which although being a complicated piece of equipment is so simple to operate that it can be used easily by people from 4 till over 80 years of age.

The above example shows the way to go. However, in industry there are also many examples that point in the direction of simple and robust designs. Currently, in The Netherlands, there are numerous applications of co-generation energy systems that are

Fig. 1.1. Domestic refrigerator.

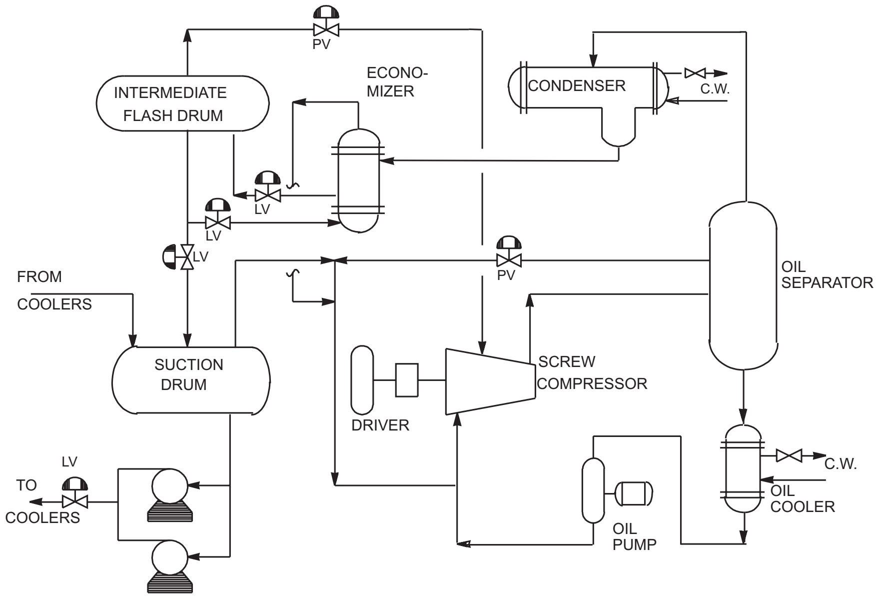

Fig. 1.2. Industrial refrigerator; technical layout.

operated remotely from a central control station. When something goes wrong, the unit may shut down automatically, while maintenance person next to the operator has remote access to the system in order to diagnose the cause of the failure.

The operation of air separation plants is also practiced by remote control, and currently this system is used by the major suppliers of oxygen and nitrogen. Other examples of remote-operated systems include: compressor stations; water treatment systems; unmanned oil platforms; and refrigeration systems – all of these are at different locations and operated by experienced companies in their field. The above-mentioned applications are not only remotely controlled – they also have to meet higher levels of reliability and safety performance in order to permit unmanned operation.

The design of these process units had to be adapted to meet high standards on safety, reliability, and operation. I was once told by an air separation engineer that in order to achieve the remote operation it was necessary to strip the instrumentation to avoid plant stops caused by instrument nuisance. The concept was:

It is better to have a few good instruments than lots of unreliable ones.

The design of chemical plants needs to make an evolutionary step if it is to approach the performance of a domestic refrigerator.

1.2 The Process Plant of the 21st Century: Simple and Robust

The characteristics of a chemical plant in the 21st century were presented by I.G. Snyder, Jr. of Dow Chemical at ASPENWORLD, November 7, 1994, in Boston, Massachusetts, USA. In his presentation, he described 10 operational paradigms to be achieved:

1. Produce a product without blowing the plant. To realize this, we must have not only a good understanding of the safety aspects of a facility and its chemicals, but also of the techniques to minimize the risks. It is clear that we need to apply the principles of inherently safer design, as advocated by Kletz (1991), IChemE (1995) and CCPS of the AIChE (1996).
2. Produce a product with instrumentation. Operation of the plant is taken out of the hands of the operator, but this requires a carefully developed and implemented automation strategy.
3. Produce a product effectively and efficiently. Design optimization plays a key role in this objective
4. Produce a product optimizing multiple variables. Management wants to stimulate all kinds of targets, such as greater throughput, less energy, higher selectivity, and less maintenance.
5. Control the plant rather than the unit operations. The design and implementation of a control system that achieves total plant control versus unit operation control. This will be the baseline for operation optimization
6. Optimization of the plant with continuous technical supervision. Operation optimization is the objective – the facility needs to run continuously against its constraints. To enable this, a multi disciplinary input is required to develop accurate process and control models.
7. Optimization of the site. The trend will go in the direction of one control room per site. Site optimization models will be available to select the operational targets for the entire complex.
8. Economic optimization of the business. Business models will be available to support business teams to select the targets for the individual plants.
9. Direct customer interaction. Customers need direct product information based on product models for product design and operation. The "just-in-time production" concept requires production flexibility, with short-term adjustments of production schedules to meet customer requirements.
10. Worldwide plant operation. Global manufactures will be able to compare and optimize on line plant performance and operation of different facilities in the world.

Another reference in this respect is "plant operation in the future" (Koolen, 1994), which defines as the objective for the operation of a processing plant,

> *Hands-off operation within safety and environmental requirements with a minimum of operator intervention at optimal process conditions.*

In this report, it was argued that such an objective had to be achieved through the development of fundamental process models, in static as well as dynamic state. The application of these models for control design as well as operation optimization is considered as apparent.

The above discussion mainly concentrates on the operational requirements of a process plant. The plant of the 21st century has more extended characteristics which should bring it close to a domestic refrigerator. The definition of the simple and robust plant for the 21st century plant, as adopted in this book is:

An optimal designed safe and reliable plant, operated hands-off at the most economical conditions.

Such a competitive plant can be achieved by striving for the following objectives:

- Plants must be captured in fundamental models statically as well as dynamically, to achieve understanding, design and operational support.
- Design optimization must be applied based on computerized flowsheet evaluations including process synthesis tools with economic objectives, respecting the safety, environmental and sustainability constraints.
- Plants should be reliable and maintenance-free, and achieve a schedule of 4–5 years between turn-arounds.
- Plants must be safe, environmentally sound, and – if required – automatically fall in a fail-safe mode.
- Operational activities such as start, stop and regeneration should be fully automatic, and be tested with simulations before actual operation.
- Control should be robust and hands-off, with an adequate disturbance rejection capability. The control design must be based on dynamic models.
- Optimized operation based on mathematical models should be performed on-going in relation to the site and the business.

Simple and robust plants are low-cost plants. The ratio of annual profit per investment is the ultimate economic performance yardstick for each investment. Worldwide, this is the basis for comparison of economic operations. The sensitivity of the economic performance for the investment in a facility is demonstrated in the following example.

$$\text{Annual profit/investment} = \frac{(revenues - cost)/year}{investment} \times 100\ \%$$

The direct fixed capital (DFC) of a process plant is 10 MM
The site-related capital is $0.1 \times$ DFC is 1 MM
Total investment is $1.1 \times$ DFC = 11 MM

Revenues are 20 MM/year
Variable cost (raw material + energy cost) are 16 MM/year

Capital-related cost:	
Maintenance cost	2 % of DFC
Operational cost	2 % of DFC
Depreciation	10 % of DFC
Capital cost	10 % of DFC
Total capital-related cost	24 % of DFC
Total capital cost related to investment	24 % × 1.1 × DFC = 26.4 % of DFC = 2.64 MM

The annual profit per investment becomes:

$$\text{Annual profit/investment} = \frac{(revenues - variablecost - .264\ DFC)/year}{1.1 \times DFC} \times 100\ \%$$

$$\text{Annual profit/investment} = \frac{(20\ MM - 16\ MM - .264 \times DFC)/year}{1.1 \times DFC} \times 100\ \%$$

which is equal to 12.36 % for a DFC of 10 MM

The sensitivity of the economic performance of the process plant as a function of the DFC is shown in Table 1.2. An additional column has been added for a capital-related cost alternative of 0.2 × DFC. This might be realized by a longer depreciation period, or a lower capital cost.

The results in Table 1.2 show that, compared with a DFC of 10 MM at capital-related cost of 0.264 × DFC, the economic performance is strongly related to the DFC.

A decrease of the DFC by 25 % to 7.5 MM doubles the economic performance to 24 %.

An increase of the DFC by 20 % to 12 MM halves the economic performance to 6 %

A similar strong relationship between profit and DFC can be concluded from the column with the lower capital-related cost.

Table 1.2. Sensitivity of economic performance versus investment.

DFC of facility (MM)	*Annual profit/ investment**	*Annual profit/ investment*+
7.5	24.48	30.3
10	12.36	18.18
12	6.30	12.12
15	0.24	6.06
20	–5.82	0.0

* % at capital cost 0.264 of DFC.

+ % at capital cost 0.2 of DFC.

The conclusion is that the profit on a project is strongly influenced by the DFC and therefor simple designs leading to low cost designs will have a strong economic interest of the businesses.

1.3
Design Philosophies

The realization of the design objectives for a 21st century plant requires a different approach to process design. Therefore, design philosophies have been developed (see below), which are elucidated in greater detail in **Chapter 3**. Prerequisites for the application of the design philosophies are: an integrated modeling environment; the properties of the components; and models of chemistry and phenomena.

Ten design philosophies were developed and brought forward from different viewpoints, and include:

- simple and robust process plants (Koolen, 1998);
- world-class manufacturing (Schonberger, 1986); and
- inherently safer and environmental sound chemical processes.

Simple and Robust Process Plants Perspective

1.3.1
Minimize Equipment and Piping

Most plants have an excess of equipment. Often, equipment can be completely eliminated or combined in function with other equipment. These pieces of equipment are selected by applying a stepwise logic performed during design. A breakthrough in the way of thinking is required to achieve this simplification step, while the process technology to achieve this, is within reach.

1.3.2
Design for Single Reliable and Robust Components Unless Justified Economically or from a Safety Viewpoint

This philosophy needs to be applied consistently to meet the objective of simple and robust design. Currently, most designs are based on the assumption that components are unreliable, and therefore redundancy is considered by default. This leads to spare provisions such as pumps, reactors or reactor systems, double or triple instruments, safety devices and others. Currently, the design of the individual components is very reliable, but many failures are caused by wrong component selection, installation and operation practices. Reliability data and reliability engineering techniques are available today to support and quantify the single component design philosophy (this will be discussed later).

1.3.3 Optimize Design

This effort can be split into optimization of the process design and of the supply chain. To pursue process optimization, techniques and process synthesis tools are available in commercial simulators. For the optimization of the supply chain (including feed, intermediate and product supply), information must be gathered on reliability and availability (with its probabilities) of feed and product deliveries, process reliability and availability (planned or unplanned) with its repair and recovery times. This can be accomplished with reliability modeling (Koolen et al., 1999).

1.3.4 Clever Process Integration

There is a trend in process design to maximize process integration. The trend set by the energy optimization is now extended with the integration of water, and hydrogen and in fact counts for all streams that are subject to re-usage. A high level of integration can result in high savings from a steady-state perspective. The disadvantages of integration are the availability of the "service" stream and its dynamics that need to be understood in all its aspects. We must differentiate between: (i) integration within a unit where we must watch for start-up and unit stability; and (ii) integration between units (processes) that asks for careful design of the system to handle disturbances and availability. Dynamic studies in close consultation with control engineering are a requirement, where provisions for de-coupling in terms of hardware and software are a requirement for robust control and operational design.

1.3.5 Minimize Human Intervention

Human beings are able to develop and exploit new things. They have – next to others – a characteristic which, depending on the situation, can be either an advantage or a disadvantage. Humans like to learn and improve, often by trial and error, but this means they are not consistent in performing tasks. For the operation of chemical plants, this is a handicap which leads to many process upsets and often must be resolved by human intelligence at a later stage. The best way to overcome this is by implementing a high level of automation for routine operations and robust control design, yielding reliable closed loop performance. Currently, most processes have an operator in a control loop to obtain the required quality of operation.

1.3.6 Operation Optimization Makes Money

Process plants are always operated in a variable business climate that has an impact on its economic operation. The variations in prices of raw materials, energy and products and their demand will have a large impact on plant's economic performance. These variations may occur on a daily, weekly or monthly basis, although there may also be variations on an hourly basis. Other quite common variations are:

- the day and night temperature cycle that might challenge ongoing maximization of the operational capacity;
- production schedules, product transients;
- raw material composition; and
- fouling or catalyst aging.

As all these variations have an impact on the economic optimum for operation, an optimization effort is more than attractive, that often justifies a closed loop optimization. The objective of the optimization is to maximize the profit of the operation. The introduction of a profit meter (as described by Krist et al. 1993) is an essential element of operation optimization. The profit meter is based on plant mass balance streams (preferably calculated by reconciliation of the plant mass balances) in convolution with the individual stream economic prices to make a continuous real-time financial balance, to support real-time optimization.

World-class Manufacturing Perspective

1.3.7
Just-in-time Production (JIP)

This concept has been developed since the early 1980s, and was focused on the production of components or a set of integrated components The principle of minimizing the feed, intermediate and product storage can also be applied in the process industry, and is fully in line with the basics of simple and robust design. The minimization of storage is accomplished through the integration of production lines and storage in transport. The minimization or even elimination of storage was in the past applied in case of low-boiling liquids or extremely hazardous materials, for example hydrogen, methane, ethylene, chlorine, and ammonia. This demonstrated that, from a logistic and a technical point of view, the techniques to deal with these situations are available. The key is the mind set to evaluate this also for other situations.

1.3.8
Design for Total Quality Control (TQC)

The concept of TQC can be divided in two different philosophies:

1. *Prevent upsets versus cure.* Nowadays, it is common practice to design process plants with many provisions for recycling, such as recycle tanks and check tanks. All these provisions are “required” to deal with any off-spec situation during start-up and “normal” operation. Next to the investment cost of these provisions, recycling of material always costs capacity and additional operational cost. On occasion, we even design the capacity of the plant to include a

certain percentage of product recycle, which results in a need for more capital. The concept of "prevent versus cure" attempts to avoid all these additional provisions. The solution is consistent operation, which can only be realized by a certain level of automation and much more attention to feed-forward control to avoid off-spec situations. Do not build a plant for all types of mishaps (excluding safety provisions) – do it right the first time.

2. *Design for first-pass prime*. This is a specific case of "prevent versus cure". During start-up of a plant, it is often necessary to deal with off-spec situations. The challenge is how to prevent these and thus avoid all the rework and/or losses. The answer is to design for first-pass prime, and this often involves designed start-up procedures. Start a continuous process from the back end, and put the finishing sections of a plant in hot stand by condition. This means that the finishing section is at operational and specification condition (e.g., distillations are at total reflux, compressors run in recycle mode) and ready to process the feed from the reactor section. In addition, it is necessary to prepare the reactor for a flying start. This requires a good understanding of the reactor operation that can be obtained from dynamic simulations, leading to start-up procedures to achieve first-pass prime. The hardware modifications to achieve this are limited, and mostly result in minor piping modifications. A leading article on this subject was produced by Verwijs et al. (1995). An example of minimization of components by total quality control and no redundancy is shown in Figure 1.3.

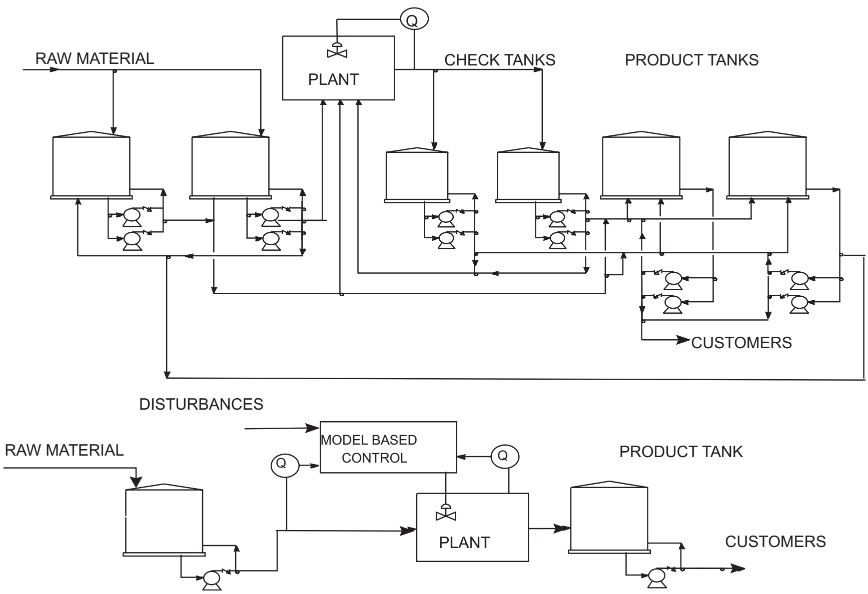

Fig. 1.3. Minimize components by total quality control and no redundancy.

Inherently Safer and Environmentally Sound Processes

1.3.9
Inherently Safer Design

This concept is based on four guiding lines (Kletz, 1991; CCPS, 1996) that were accepted as bases for design by IChemE and the CCPS of AIChE. The approach intended to minimize the risk of a facility through the minimization of hazardous situations. The key words are; minimize, substitute, moderate simplify.

Minimization of hazardous material This can be realized by storage minimization which is also in line with JIP. The application of gaseous feeds versus liquid feeds should also be considered. This can be a realistic option in case of low-boiling point materials such as chlorine, ammonia, and phosgene. The reduction of inventory in the process is an opportunity, like the removal of a reflux drum in a distillation column or application of column packing versus trays.

Substitution of a chemical with a less hazardous material There are many examples of substitution, including: (i) the selection of a different material – perhaps to replace a strong acid with a weak acid, or a toxic material by a less-toxic equivalent; (ii) the dilution of a material; and (iii) the selection of a different physical phase, possibly from solid to solution.

Moderation of hazardous conditions This might be carried out in order to minimize the impact of a release of hazardous material or energy (this is also known as "Attenuation" or "Limitation of effects"). Different options that might be considered include operation at less harmful temperature, pressure, concentration and phases, and the avoidance of interaction of chemicals.

Simplification of a facility This would be conducted from an operational point of view in order to avoid operational errors. Items that have a major impact on the level of complexity include:

- Piping connections: more connections provide opportunities for misunderstanding, more operator interventions, and potential errors;
- Degrees of freedom (DOFs) for operators: more DOFs give more operational variables to the operator. All manual valves, switches, controlled and manipulated variables, and analog outputs AOs with manual over-rides are DOFs, with opportunities for errors and disturbances. The DOFs can be reduced by a higher level of automation, in combination with the minimization of valves and manual over-rides.
- Interaction of the process with other sections or external sources, static as well as dynamic. De-coupling of the interaction through hardware and software solutions (robust control) can solve this.

1.3.10
Environmentally Sound Design

Nowadays, although the chemical industry operates increasingly on a global scale, the environmental criteria applied in different countries vary widely. Many global criteria and trends are introduced first in the Western world, but in time become readily accepted throughout the rest of the world. A relatively new term in that respect is “sustainability”, and this needs to be addressed adequately during the design. For a new facility, this means that the design should increasingly meet global criteria, rather than local criteria.

1.4
Process Synthesis and Design Optimization

These are the most important stages during the design as they determine the flowsheet and its sizing, and therefore set the bases for the economics of the process (see **Chapter 4**). In the past, different hierarchical structures have been developed, such as the well-known “onion model”. The drawback of the proposed schemes is that the level of interaction is unsatisfactorily addressed. Therefore, another hierarchical structure for conceptual process design is presented, and this is referred to as the “interactive onion model”. The design starts from a feasible flowsheet(s) with alternatives, and concludes step-wise to one frozen mass and energy balance, with all major equipment sized. The steps are described, and in particular the interaction with process integration and controllability are include in the structure. Guidelines are included to avoid complex integration and to de-couple interactions through hardware or software solutions.

Specific attention is given to the optimization effort – a staged approach – which is applied during the process synthesis methodology, starting from the evaluation of a large number alternatives for the different sections against variable cost. Finally, the ultimately selected flowsheet is fully optimized with regard to conditions and equipment sizing at NPV (net present value). It is considered to be an advantage that the designer can follow the gradual development of the flowsheet, simultaneously monitoring the different optimization stages while increasing the modeling details.

1.5
Process Simplification and Intensification Techniques

The emphasis in **Chapter 5** is placed on technical aspects of process simplification and intensification. Process intensification is driven by the same objectives as simplification and cost reduction, and therefore both are discussed. The difference is in the approach, with intensification being focused primarily on the decrease in unit size by application of improved techniques, while simplification benefits from existing techniques.

Design techniques to achieve low-cost processes may be divided into different categories:

- Elimination of functions
- Combination of functions in the same unit/equipment
- Integration of equipment
- Intensification of process functions
- Overall process simplification

The opportunities need to be recognized during the conceptual design stage. The details of the different categories will be presented and illustrated with examples in **Chapter 5**.

In order to make simplification and intensification more easily approachable, opportunities are presented for the most common process units, including that of piping design. The examples will clearly illustrate what can be achieved by application of this method. The chapter concludes with a debate on any contradiction between simplification and further process integration.

1.6
Design Based on Reliability

Reliability engineering is one of the pillars of simplification, and is based on the philosophy, "Design for single robust components unless ...".

The technique of reliability engineering is discussed in **Chapter 6**, together with its application in the design of process plants. The text provides a quantitative basis for any design decisions around the installation of more parallel units (provisions) as back-up, or the installation of more reliable units. The same technique can also be applied to evaluate instrumental safe guarding, and to estimate nuisance trips due to instrument failure. Although the mechanical reliability of process units is improving, the number of nuisance trips is increasing as a result of instrument failure. This is also due to the tendency to add more and more instruments to the process. Reliability engineering also provides a quantitative base for risk analysis with regard to the likelihood of an event. It should be realized, however, that all predictions on the probability of failures are based on historic data, and this is not a guarantee that newly designed components will always meet these criteria. For example, the motor industry suffers from this phenomenon if certain components are replaced by new alternatives.

1.7
Optimization of a Complex, and Evaluation of its Vulnerability

The optimization of a complex – which might be a chemical complex, a refinery or a number of food processing plants sited at one location – will be discussed in **Chapter 7**. The investments in logistic facilities and services at a complex are very high. The design philosophies for a complex of processes are presented, and on the basis of these a quantitative methodology based on reliability engineering techniques is shown to optimize the logistics of a complex. The vulnerability of a complex can be quantified through the development of a reliability flowsheet of its different sections/processes, including utility generation and external supplies. The vulnerability of a complex can be evaluated and its potential losses quantified and compared with alternatives, which include back-up provisions, sizes of storage, or improved reliability of units.

1.8
Design of Instrumentation, Automation and Control

The design of the automation and control are essential elements to comply with a process that is operated hands-off, and under the most economical conditions. To realize this objective, attention is given in **Chapter 8** to the design of all the elements that contribute to it. An empirical approach will not be sufficient to achieve the level of robustness; rather, a dynamic simulation will need to be made available in order to enable the design.

The *instruments* are the eyes, ears, and hands of the process, and special emphasis must be given to them. Firstly, they need to be measuring correctly what we want to measure in terms of the process condition. This seems straightforward, but how often do we measure a volumetric flow that is influenced by density or temperature when we are really interested in a mass flow? Other important aspects of instruments include: range, accuracy, reliability, robustness, in-line measurement (avoid sample lines) self-diagnostics, installation, and calibration. All measurements should provide the correct information so that the process's organs of sense "see" what is happening and automation and control systems can take the correct action.

Nowadays, automation of operation is making extensive progress in terms of implementation. As automated process become more consistent in executing tasks, the result in turn is more consistent production. However, a major question to be addressed is, "how far do we want to go with automation with regard to the role of the operator?" How do we keep the operator alert and responsive during the operation? Currently, a number of quantitative investigations are under way to cover this point. However, one important aspect of simple designed process is that, by increasing the level of automation, the DOFs of the operator are not reduced and the system made less complex from operational perspective, (**Chapter 2**). This assumes that the operator does not have all kinds of manual over-rides. The surveyability of the process is another important aspect for a good man–machine interface, to support the operator in case he or she has to interfere with the operation.

Robust control design is one of the most difficult tasks, notably because the requirements for product quality, environmental and safety are increasing, while the interaction and response times also have a tendency to increase, due to a higher level of integration. The approach for the design of control configuration is presented in **Chapter 8**. In the past, control design was an empirical effort, but current control strategies and controls must be designed based on dynamic simulations, and have to meet the criteria of hands-off operation. The design of the control strategies must be based on integral process operation versus unit operation. (Luyben et al 1998).The design principle followed is that an operator should be able to run the operation using the basic control layer at specification. Any outage of a higher level control layer or optimization layer should not result in process outage, although it might run less optimally. In order to anticipate interactions, it may be necessary to build hardware and software provisions that uncouple these effects. All of the above points must be fulfilled if robust control is to be achieved.

1.9 Operation Optimization

Operation optimization has been used for some time now, especially with regard to scheduling for batch plants, or linear programs for refinery operations.

Currently, off-line programs based on non-linear programming (NLP) techniques are the state-of-the-art for feedstock evaluation and selection of the most economical conditions for chemical plants on a daily basis. One precondition however, is that there is a reasonably accurate reactor model.

Closed loop static optimization for continuous plants based on non-linear techniques is a recent (within the past decade) development that required a robust control design and an implementation methodology. Forthcoming developments concentrate on the dynamic optimization of product type changes and cycle time optimization of batch operations. In this respect, they also include the cycle time optimization of gradually degrading/fouling systems of continuous plants. The optimization options and methodologies for implementation are discussed in **Chapter 9**.

1.10 The Efficient Design and Operation of High-quality Process Plants

During the preparation of this book, two questions with a general theme were received regarding the implementation of simple and robust designs:

1. How can existing processes be improved?

2. How can this be implemented in a project in order to achieve high-quality designs and operation?

These questions will be addressed in **Chapter 10**, where the operation and continuous improvement of an existing plant is discussed, notably with regard to the following points:

- process capacity upgrading;
- process reliability and availability;
- quality of operation;
- operation optimization; and
- identification of design improvements.

The efficient design of high-quality plants is presented along two lines: (i) the elements required to design a good work-process (methodology) for process design; and (ii) the essentials to assure the quality of a process design.

In order to achieve quality designs the chemical industry introduced Value Improvement Practices (VIPs), the implementation of which during the design is crucial for the quality. The VIPs might be different for different companies, but incorporate the following topics:

- technology selection;
- waste minimization;
- process simplification;
- process and energy optimization;
- reliability modeling;
- design to capacity;
- maintenance;
- construction; and
- value engineering.

Functional analysis is an essential technique for the implementation of process simplification. The technique, which was developed as a tool for value engineering (Snodgrass and Kasi, 1986), began in the 1970s and 1980s to force the weapons industry in the U.S.A. to deliver at lower cost. The same technique can be applied to the introduction of process simplification in the process industry, and is incorporated in the VIPs, simplification and value engineering.

1.11
Overall Example of Process Design

Having briefly described these design philosophies and techniques, an example of the evolution of a batch process from its initial design, and its development to a simple and robust design, is provided. A typical batch process is illustrated in Figure 1.4, as it was scaled-up from the preparation at laboratory scale. In this example the chemicals are introduced in the reactor vessel at the beginning of the planned reaction, and all successive treatment steps are executed in the same reactor vessel. Batch reactors may be used for all types of chemicals and treatment steps. For example, the following treatment steps can be mentioned: post reaction, neutralization, distillation, evaporation, devolatilization, extraction, crystallization, cooling, washing, filtering, drying and additions for customer processing and product inhibitors.

Typical for original designs for batch processes is the initial loading of the reaction components and the opening of the reactor vessel to add chemicals manually. Such a process has several handicaps; initially, it is less safe, as pre-loading of the reaction components may result in an uncontrolled reaction. Another disadvantage

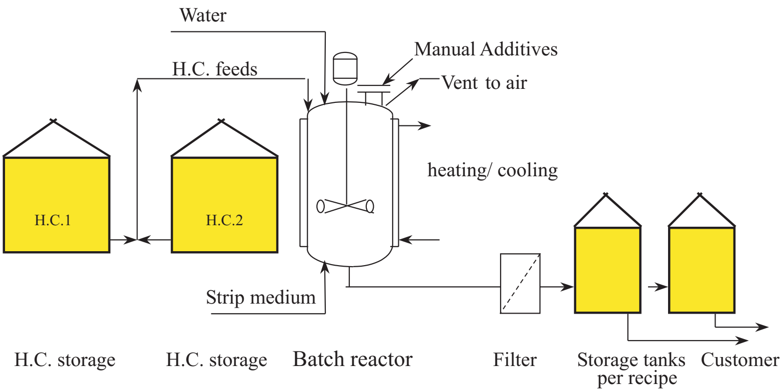

Fig. 1.4. First-generation flowsheet of batch reactor plant with an extended product tank park.

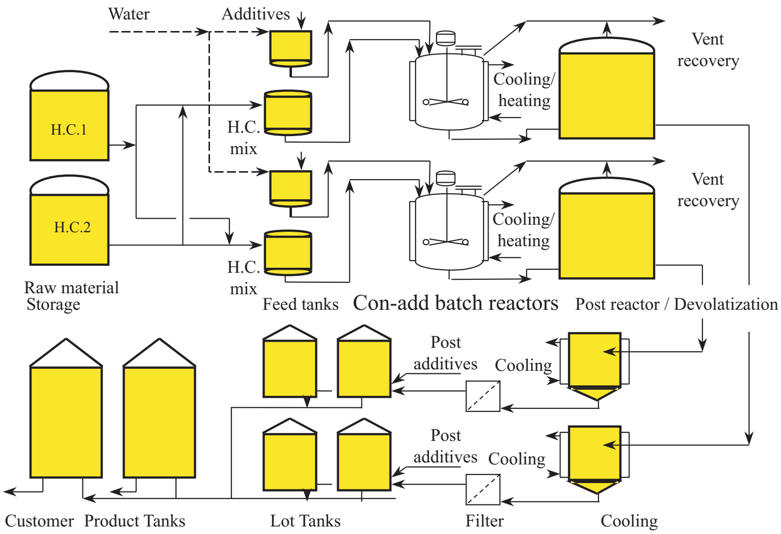

Fig. 1.5. Second-generation flowsheet of continuously added batch reactor systems: safer, and higher capacity.

is the opening of the reactor, which brings operators into direct contact with chemicals and introduces air into the reactor vessel – a situation which is often undesirable. The size of the reactor was limited due to fabrication limits and the limited cooling capacity for jacketed vessels. A larger vessel diameter increases the volume with the cube of the diameter, while the surface area increases with the square of the diameter.

The second generation of this batch process is shown in Figure 1.5. The reactor is provided with continuous feed streams to establish a more constant heat generation during the reaction feed step. To accommodate this, feed vessels are installed in front of the reactor vessel. Opening of the reactor vessel is avoided by adding the ingredients into harmless feed systems, or separate dosing systems are installed to supply the additives. Following the reactor in this example, a post reactor is applied, and de-volatilizing and cooling is carried out in separate vessels. The product is intermediately stored in lot tanks to equalize the product, followed by storage. The flowsheet represents a large increase in capacity by providing additional equipment where the feed preparation and treatment steps are carried out, while the process is automated. The additional equipment was in general justified based on incremental economics. The reactor vessel was reserved for the reaction alone. Larger reactor vessels could be applied (which by that time could be fabricated) due to the improved control of the heat generation. Two reactor systems are shown to cover the increased demand.

In the third-generation process, feed is applied directly to the reactor vessel, while the reactor size is increased by the application of a reflux condenser, though it still

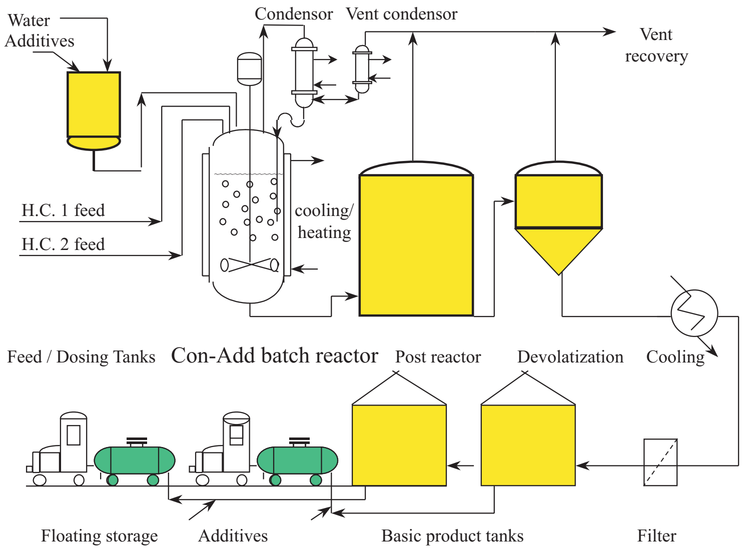

Fig. 1.6. Third-generation flowsheet of continuously added batch reactor system with refluxing condensor and floating storage.

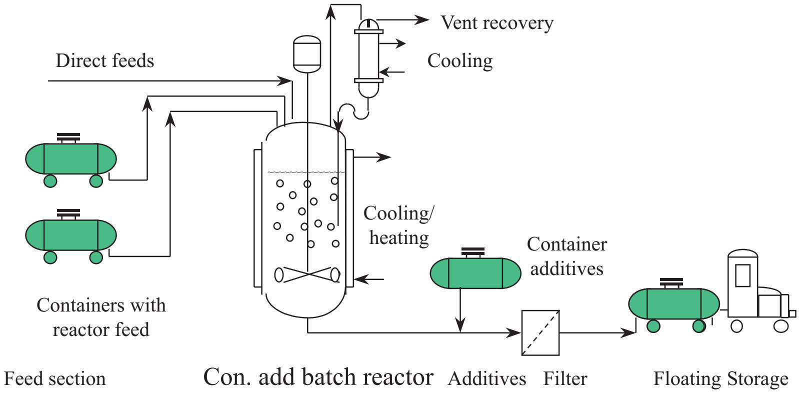

Fig. 1.7. Flowsheet of a simple and robust batch plant.

has a post reactor. A continuous finishing was foreseen and removal of the lot tanks, while basic product storage was provided (Figure 1.6). The system became considerable cheaper also as only one reactor system was required to cover full capacity versus the second generation system which had more reactor systems.

The ultimate flowsheet of a simple and robust batch process is shown in Figure 1.7. The design philosophies as discussed above were applied, and the reactor may be used for several types of operations. All storage facilities are removed. Additives are supplied from containers before loading of the transport container for shipment to the customer. Even services such as refrigeration and heating might be obtained from suppliers who operate remotely and maintain services on the location. Adequate control of the reactor and the feed and dosing systems is required. The capital of the process is significantly reduced per ton of product

Simplification of a distillation train also has considerable opportunities. The relative boiling points from the components before and after the reaction are shown in Figure 4.16 in **Chapter 4**. The conventional design is shown in Figure 4.17 starting with five distillation columns. The evolution is illustrated in Figures 4.18–20. The advantages of combining more distillatory separations in one column leads to considerable savings, and this is reflected in the reduction from five columns to two – a real advertisement for simple design!

1.12 Summary

The plant of the 21st century has to change its design concept and is defined as:

An optimal designed safe and reliable plant, operated hands-off at the most economical conditions.

This concept has been developed and applied in its ultimate form in a domestic refrigerator, but also at remote locations such as drilling platforms and air separation plants. A simple and robust plant has considerable cost advantages, usually in the order of 30–40 % on investment. The design philosophies and techniques necessary to achieve this are presented in a general form. The methodology for implementation is an essential step for the realization of the concept, and will be discussed later in detail.

The design aspects and specific design techniques are mentioned, while the operation optimization is the way to maximize operational profits. Optimization of an integrated complex is to be discussed, while the quantitative methodology for the evaluation of the vulnerability of the complex will be presented.

The evolution of a batch process and a distillation train is shown from its initial design through several generations up to a simple and robust design.

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Chapter 2
Simple and Robust Plant Design

2.1
What is "Simple"?

Definition: a system or device is simple if the user understands its purpose and is able to operate it with few manipulations, while any wrong or unstructured manipulation will not result in any damage. Restart of the system should be easy and realized with one-button operation, while the safe guarding should result in a fail-safe situation

Some examples will be used to explain simplicity. Electrical lighting is a simple device: the user understands its function of "light", and its operation with a single switch. The safeguarding is done with a fuse. If the bulb does not light, the user action may be to install a new bulb, but all other actions are for an "expert". Another example is the water reservoir of a toilet cistern, which has a level control for the water supply. The water level in the reservoir is automatically kept constant through a level-actuated valve in the water supply. The reservoir has an overflow protection to a safe location. If the system does not flush, the user understands that he/she must call for assistance, because they know that the basic function of flushing is not available. A third example is a television set: even elderly people understand the function of the device and its three basic operational functions (on/off switch, program selector, and volume button). The fact that many TVs have a complicated handset is a problem that some suppliers are solving by hiding function under a special cover, or by using a special color for the essential buttons (Freudenthal, 1999).

The above examples show devices that are simple for the user to operate, but on the other hand they can be very complex for the designer, the manufacturer, or maintenance person. Just consider the difficulties and complications involved in the design and manufacture of a TV set!

Let us compare this situation with some process plant details. For example, a line connects two vessels with the purpose of transporting liquid from vessel A to B (Figure 2.1). When this line is introduced, we need to have back flow protection. The standard solution for this is a check valve, although we know it will always leak and so it is not fail-safe. A solution in such a case is always to keep the up-flow vessel at a higher pressure then the down stream vessel.

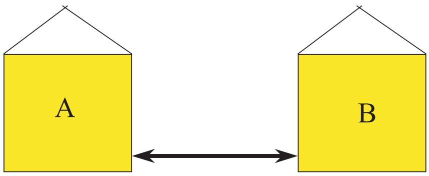

Fig. 2.1. How to protect back flow.

In that case we normally have two pressure measurements converted in a pressure difference, and a control device with an actuated shut-off valve. This is independent from any pressure protection (low and high) on the vessels, and from any flow device to control the flow. The tank shown in Figure 2.2 has 10 possible connections, and in case of any change in level it will be difficult to analyze the cause. To illustrate this, consider a set of manifolds with a number of flow interconnections (Figure 2.3). One single line has only two flow interconnections from vessel A to vessel B and vice versa. In case of a manifold of seven connections, there are already 42 flow interconnections. The number of flow interconnections in relation to the connections of a manifold is described as:

$$\mathrm{I} = 2 \times \sum_{i=1}^{i=n-1} (i-1), \tag{1}$$

where I is number of flow interconnections, and i is the number of connections.

We can list this for the number of flow interconnections as a function of the number of connections in a manifold (Table 2.1).

It will be clear that when the number of connections increases, the number of potential errors in lining up and eventual error detection points increase steeply. Of course, not all manifolds are as complicated as this, and when one considers a steam header system, the situation is often designed in such a way that there is one high-pressure inlet and all other connections have a low pressure. This prevents back flow and also considerably reduces the number of potential flow interconnections.

When we compare a TV set with a piping manifold, it might be concluded that a TV set is a simple device because everybody understands its function, and even

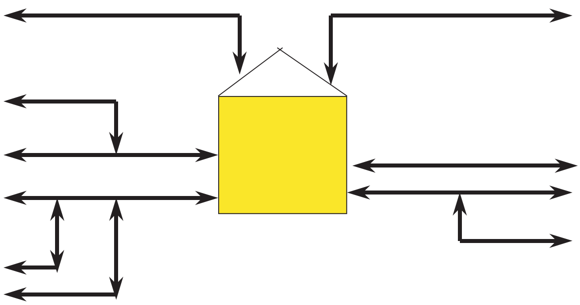

Fig. 2.2. Vessel with ten connections, what causes the increase in level?

elderly people can operate it. On the other hand, it is a very complex system to design and manufacture. By contrast, the manifold is a very simple device to design, but very complex to operate. It is essential that the conditions of all connecting vessels are known for a correct operation, and it is difficult to analyze for error detection.

In the above text, "simple" was defined from an operational perspective (easy to operate), but this does not have any relation with the complexity of the device/system. It will be understood that the operation is simplified when less degrees of freedom (DOFs) are available for the operator. In practice, this is realized by the introduction of automation, as a higher level of automation reduces the DOFs for the operator.

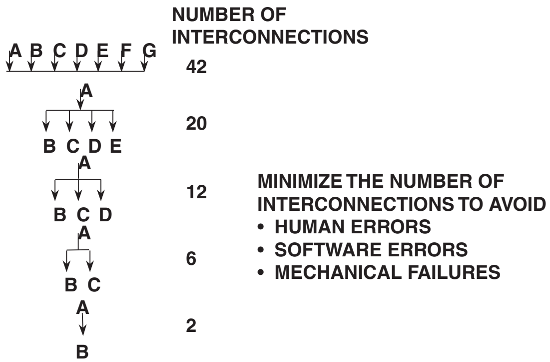

Fig. 2.3. Manifold with the number of flow interconnections

Table 2.1. The number of piping connections versus the number of flow interconnections.

No. of connections	*No. of flow interconnections*
1	2
3	6
4	12
5	20
6	30
7	42
8	54

2.2 The Level of Complexity

The term "complexity" is introduced when a total system is considered. It was Scuricini (1988) who defined the complexity of a system as:

A system is complex when it is built up of a plurality of interacting elements of a variety of kinds, in such a way that in the holistic result no evidence can be traced of the characteristics of single elements.

The factors that determine complexity are (Scuricini, 1988; Wieringa and Stassen, 1993):

- the number of components;
- the number of interconnections;
- the number and level of interactions; and
- the variety of components.

From an operational perspective can be added:

- the number of measurement readings;
- the DOFs for the operator; and
- the surveyability of the state of the system.

The above are explained by example of a unit operations which have as their objective the achievement of a certain reaction or separation. These operations are composed of a set of components. For example, a distillation column often has a tower, reboiler, condenser, reflux drum, and pumps, with installed spares for feed, bottom and reflux/distillate flows next to its piping and instruments. The total number of equipment pieces can be 10 – or even more if we add cross-exchangers, additional reboilers, and vent condenser. With regard to the design, we already have quite a few different components, with several interconnections adding to the complexity.

For a standard distillation in its operational step there are six controlled variables, all of which are DOFs: feed, pressure, top and bottom specifications and the levels in the reflux drum and the bottom of the tower. Depending on the control strategy, each controlled variable will have a selected manipulated variable, which include setpoint settings. The total number of manipulated variables, which include manual valves, for start-up/shut-down and exchange of pumps is much greater. The total number of DOFs for the operator will add to the complexity.

A process plant is a set of unit operations connected to each other. A simple process plant can have sequential unit operations (Figure 2.4) where the flow goes from unit A to unit B, and successively to unit C. This might be compared with the toy train that a child play with: as more and more carriages are connected to the train it does not add to the complexity of the operation, because for the train driver the operation is still the same. The sequential operation might be compared with the situation shown in Figure 2.5, where the same main flow line exists from unit A to B to C. Now, there are also a number of cross-connections between the different units, and clearly these interconnections will add to the complexity. All these connections are a source for disturbance and interaction. From the operation perspective the DOFs increase, but so too does the number of disturbances and interaction increase for each unit. In the sequential operation example there were only disturbances from the upstream and downstream units.

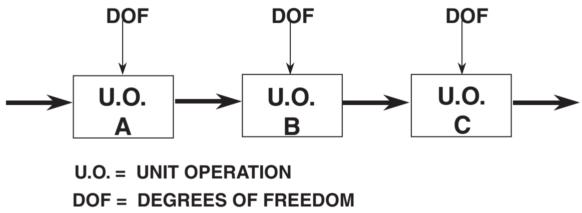

Fig. 2.4. Sequential operation.

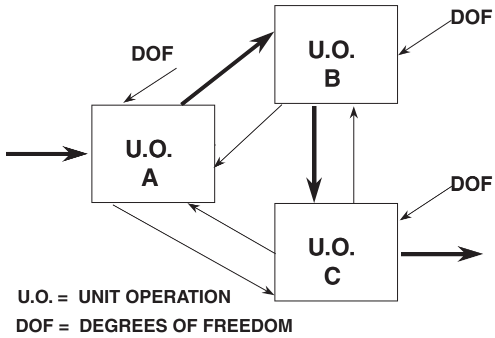

Fig. 2.5. Sequential operation with interaction.

In the example of the distillation column the disturbances are introduced through feed stream, heating and cooling media. Interaction is inherently part of the distillation system as the quality controllers of the products impact each other.

Based on the overall definition of complexity, a specific complexity can be composed for a unit operation in a chemical process plant.

The level of complexity, C, of a unit in a chemical process is defined as a function of:

- M, the number of equipment accessible by the operator;
- N, the number of DOFs, including manual/actuated valves/switches and set points of control loops;
- O, the number of measurement readings;
- P, the number of input and output streams, including energy streams;
- Q, the interaction in the unit requiring an operator intervention; and
- R, the number of external disturbances (for the unit) asking for action from an operator.

Note: For Q, under interaction we understand that if, an operator manipulation is performed to achieve a certain change in a controlled variable, at the same time another controlled variable is strongly influenced that would require another operator manipulation to offset this change. In case the interaction is properly de-coupled in a model-based controller, it will no longer be regarded as an interaction discussion.

In formulae form: $$C\ \text{unit} = f(M)\ (N)\ (O)\ (P)\ (Q)\ (R), \tag{2}$$

where C is called the complexity factor of the unit. By summation of individual factors and adding a weight factor for each term, we have the following formulae (the impact of interaction or external disturbance may be larger than the effect of an additional valve):

Complexity becomes: $C\ unit = mM + nN + oO + pP + qQ + rR,$
where m, n, o, p, q, r, are the weight factors per item.

In generic terms: $$C\ unit = \sum_{1}^{n} a_n A_n, \tag{3}$$
where a are the weight factors and A the items.

A specific term can be further split up if we want to give different weight factors within a term. Let us look at the manipulators N: these consist of manual valve W, actuated valves in general connected to control system X, switches DOFs Y, set points Z, the respectively weight factors are in small letters.

$N = wW + xX + yY + zZ$ in generic terms $N = \sum_{1}^{n} b_n B_n,$
where b are the weight factors and B the manipulators.

Equation (3) can be simplified by using 1 as the weight factor for all terms. Thus, Complexity is now simplified to: $C\ unit = M + N + O + P + Q + R$

In generic terms: $$C\ unit = \sum_{1}^{n} A_n \tag{4}$$

Now, we can calculate a complexity number for a unit. Some examples for quantification of complexity are as follows:

- For a household refrigerator M = 1, N = 2 on/off switch and temperature set point, O = 0, P = 1 electricity, Q = 0, R = 0. Now the complexity is C = 4.
- For a simple TV set M = 1, N = 3 on/off switch, program selector and volume, O = 0, P = 2 electricity and signal cable, R = 0. Now the complexity is C = 5
- For a manifold with seven branches with its connecting equipment and the limitation of only one single line up at the time, M = 7, N = 7 number of valves, P = 14, Q = 0, R = 0. Now the complexity is C = 28

For a normal distillation column a P&ID was analyzed. With regard to the manipulated items, the following were excluded: instrument valves, blinds, safety devices. Included were vents and drains.

The values of the different terms are: M = 9 (tower, reflux drum, reboiler, condenser, vent condenser, two reflux pumps, two bottom pumps); N = 89 (control valves 7, manual valves 67, DI/DOs 9, control loops 6); O = 28; P = 12 (feed, bottom, distillate, vent stream, steam, condensate, cooling water in and out twice, electricity twice); Q = 2; and R = 3 (feed flow, feed composition, cooling water temperature). So, the complexity for the selected distillation column is: C = M + N + O + P + Q + R =143

For a process plant, which is a summation of individual units, we can add up the individual complexity factors:

Complexity of process plant: $$C\ plant = \sum_{1}^{n} c_n C_n \text{ units}, \tag{5}$$
where c_n are the weight factors per unit.

In the above formula a weight factor is introduced per unit. This might be used if we have to deal with identical or similar units operations. For an identical unit, 0.1 might be used as weight factor, and for a similar unit with the same physical separation 0.2, while for a similar unit with another physical system to be separated the weight factor would be 0.5.

It should be realized that particular interactions and disturbances in a process plant can be a severe handicap, and that this should properly be reflected in the weight factor. In these situations, weight factors of 10 might be applicable.

Weight factors have been chosen arbitrarily, and listed in Table 2.2. Those components/units that have identical or similar functions have received a lower weight factor.

Table 2.2. Weight factors for different items.

Item	*Weight factor*
Identical unit	0.1
Similar unit for the same application	0.2
Similar unit for another application	0.5
Identical measurement in radial position of vessel	0.1
Interaction with direct single relation	5
Interaction with multiple relation	10
Disturbance with simple clear correction	5
Disturbance with multiple corrections	10

We have now introduced a complexity factor that can be used to compare different designs.

When we analyse the formula it is clear how we can reduce the complexity of a unit. The answer is to reduce the individual terms such as equipment, manipulators, input and output streams, and measurements, and thus achieve a higher level of automation and control. Under these circumstances the DOFs, interaction and disturbances are reduced, and in principle a unit can offer single-button operation. An example of this might be a burner management system, which is operated hands-off while the operators do not have access to the parameters or the manipulators, as all the software is protected. Another example might be a refrigeration unit which is operated totally hands-off, with only a start/stop button being available. Any other level of action is taken by nonoperational people.

Future investigations are required to address the relationship between complexity and weight factors more accurately. In addition, the span of control of operators as a function of complexity needs to be addressed (Wei Zhi-Gang et al., 1998; Stassen et al., 1993). This might be a basis for deciding how far we should go with simplification in order to make one operator responsible for the operation/supervision of more units. Another side to the problem is that the minimum activity level of operators required to ensure correct, attended operation needs to be defined.

2.3
Why Higher Reliability?

Reliability is defined as: *the probability that a component or system performs its function over a projected time period if used in a proper way, given that the component or system was to be considered new at time zero*.

The "projected time period" used in process plants must at least meet the time between turnarounds for repairable components, while for other components their lifetime might be applicable.

The "proper way" means usage within its design limits.

The achievement of reliability is becoming increasingly important, and incorporates facets such as:

- savings on maintenance cost;
- longer standing times of components, up and until the time between turnarounds (4–6 years) to increase plant availability; and
- design for single components (capital saving and simpler designs).

The mechanical reliability of components is increasing as a result of evolution. Nowadays, vendors not only receive requests regarding the reliability of components, they also sometimes are responsible for maintenance of the equipment supplied. Situations also occur where vendors deliver services such as refrigeration or (co-)generation of energy. These companies – who historically are often suppliers of the equipment – deliver this type of service logistical spread over a large area. Their services might include:

- an operational contract;
- a minimum defined reliability and availability level; and
- a maintenance contract.

This means that it is in the company's own benefit to install more reliable components and units in order to suppress operational, unavailability and maintenance costs. These are opportunities to invest in more reliable components.

A striking example is the development of more reliable jet engines for airplanes. Nowadays, the new designs of airplane are equipped with two engines for long-distance flight over the oceans, whereas in the recent past, four engines were considered the standard. These newly designed aircraft, as well as being considerably cheaper to operate, needed to achieve the same reliability level as the older designs, and this could only be achieved by designing more reliable engines.

Another example is the considerable improvement that has been achieved with rotating equipment such as compressors. One such development was the introduction of gas seals as replacement for liquid seals, while another more recent development has been the introduction of screw compressors where neither the screws nor gears physically touch each other. In this situation, each screw has its own electric driver where the driving frequency has been synchronized very accurately.

That reliable components can be built and operated is also seen in a domestic application such as a central heating system. The heating system circulation pump is a rotating device that is installed without spares, and has a very long stand time, without maintenance.

Developments in the seals of centrifugal pumps is another good example of an evolving device. Next to the requirement for higher availability and reliability, the development was also driven by a need to reduce environmental load. This all began with the stuffing boxes, followed by liquid seals as labyrinth seals, single mechanical seals, and double mechanical seals. The introduction of seal-less pumps (and lately of gas seals) has provided a clear demonstration of how to achieve higher reliability and availability, and lower environmental loads. Similar developments relate to bearings, the evolution of which has included greased journal bearings, hydraulic jump (oil lubrication) bearings, rolling bearings, life-time greased bearings, and no-contact bearings (electromagnetic bearings).

The progress made in the mechanical reliability of components and units makes the introduction of the design philosophy "design for single reliable components unless ...", as well as the concept of "... maintenance-free operation ..." become reality. Techniques of reliability engineering which help cope with the uncertainties of reliability and its probability in design have been published (Henley and Kumamoto, 1992; Leitch, 1995; The "Red Book", 1997). In addition, reliability modeling can be performed using standard tools such as the software "Spar" (Malchi Science, Herzliya, Israel; Clockwork Design, Inc., Austin, Texas).

At present, the market has been opened up for RAM (reliability, availability, maintenability) specifications of critical equipment and supplies and services.

2.4 What is Robustness?

Reliability, which was discussed in the previous section, has been defined as "... *the probability that a component or system performs its function over a projected time period if used in a proper way*".

Robustness, however, is defined as "... *the property of a component to remain healthy and operable if it is not utilized in a proper way for a certain time*". (Note that "wrong usage" is purposely excluded here).

Robustness might be achieved in two different ways: (i) the component is resistant to improper usage; or (ii) it is made less likely to occur. In general, we prefer to have reliable and robust components, but robustness is difficult to quantify, and may be better envisaged by the help of some examples.

Many men use an electric razor that is very reliable, but when their hands are wet they might drop the razor onto the floor, where it will break. This problem has been solved by most razor suppliers by covering the hand-grip with small rubber nipples to make it less slippery. The casing of the razor also has a certain shock-resistance to reduce the likelihood of damage if dropped. In the same way, the design of a chemical complex must be prepared for mis-operation, as well as for failures of equipment and instruments. Apart from the safety provisions which must always form part of the design, we can anticipate any mishaps that might occur under the umbrella of "robustness" – which in itself can be subdivided into several types: mechanical; control; and operational.

2.4.1 Mechanical Robustness

First, we have to consider manual, incorrect operations that challenge mechanical robustness, for example the wrong lining up of a pump. For instance, an operator may forget to open the suction valve, leading to cavitation of a pump, but it is unclear whether the pump is sufficiently robust to withstand this operational error for a short period. Numerous other examples exist where the robustness of the design has been improved. In the past, many accidents have occurred because plug valves were equipped with handles, which incidentally were opened, but today most of these are equipped with hand-wheels. Another example is the casings of pumps which, in the past were often designed from cast iron – a material which cannot withstand thermal shocks. Nowadays, pumps that may be exposed to fire are designed from cast steel. The design of piping also provided the knowledge that ASA flanges are more robust than DIN flanges, and resulting in less leakage. By contrast, the selection of API pumps (which are known for their heavier construction) for standard applications did not show any major improvement in performance compared with ANSI pumps.

In general, mechanical robustness is reflected in the selection of equipment, piping items and instruments, but is also applied in control terminology.

2.4.2 Control Robustness

The term "robust control" infers that a process is able to recover from set-point changes and disturbances within a wide range, and achieves set-point tracking and disturbance rejection to its target values within a reasonable time frame. The disturbances considered are mainly changes in feed rates or composition, utilities and environmental conditions. Interruptions in conditions as trips are seldom considered under robust control. A good control design must achieve a certain robustness due to the most likely disturbances.

2.4.3 Operational Robustness

The term "robust operation" might be used for the implementation of:

- Automatic start-up, shut-down, and implementation of regeneration sequences.
- Recovery of situations where interruptions such as pump trips or alarms must be anticipated. Such situations must be foreseen and result in an automatic actions, either in process recovery or end-up in a defined standby con-

dition. Recovery might be applicable if a standby unit/provision must be started for automatic kick-in. The process actions are planned to be taken before any safety device is activated.

A strategy for the design of operational software needs to be available, and followed, see **Chapter 8**. This to ensure consistency in the automation of all units and processes, particularly if they are under the control of a single operator.

The instrumentation of the process is a major contributor to control and operational robustness, and in the field of measurements major shortcomings are a frequent problem, including:

- measurement selection;
- type selection;
- operating range selection;
- installation; and
- calibration.

The above points are independent of mechanical robustness, and address the instrument robustness as a function of the process. An example worth mentioning here is the selection of a flow meter. Often, a volumetric flow meter is selected even though the intention is to measure mass flow. The mass meters are automatically corrected for any density differences, which includes the effect of concentration, temperature or pressure changes. They measure what we want – so why don't we select them as a standard?

Instruments are the eyes, ears and hands of the process plant, and are vital to the process. Therefore, an experienced instrument engineer should be present on a project team from the process design phase until full operation to cover all facets of the instrumentation.

Although the design of the facilities needs to be considered from the perspective of robustness, this is a reasonably undefined area and hence can lead to pitfalls for those who prefer to save on capital but may lose on profit. The challenge is to recognize the likely mishaps and select the adequate component design.

2.5 Summary

The challenges for the chemical industry are to design facilities much more simply, hence making them much cheaper and easier to operate. Simplicity in design can be understood from developments in domestic equipment, and must meet requirements for ease of operation.

The level of complexity is a measure of the simplicity of a facility. A formula has been derived to quantify the level of complexity, and this can be applied on different plant designs to compare their complexity. The terms that define complexity also provide a means for its reduction.

Reliable components are an essential part of simple designs. Suppliers in the process industry have made great progress in the development of mechanically more reliable components with long stand times. The design philosophy *"design for single reliable component unless ..."* can be applied, but must be supported by reliability modeling calculations for which tools are available. The specifications of critical supplies and components need, as a standard procedure, to include reliability, availability, and maintainability (RAM specification).

In concert with more reliable components, the components should also have a certain robustness to stand or prevent likely mishaps. Different forms of robustness are recognized: mechanical, control, and operational. Robust control and operation have to absorb disturbances. It should be standard practice to incorporate disturbance rejection capability in the control design.

The design of instruments should receive special attention, as these are the eyes, ears, and hands of the process. Essential among these are: the selection of the measurement, the type of instrument, its operational range, installation, and calibration, in addition to its mechanical robustness.

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Chapter 3
Design Philosophies

In this chapter, the 10 developed philosophies are discussed to achieve simple and robust design and operation. The prerequisites before these philosophies presented are: process knowledge; material properties; and modeling capabilities. A process can designed, if a process technologist has the following tools and information available:

- Physical, chemical, environmental, health and safety properties
- Modeling environment and unit models

In this chapter, these topics will be discussed in a condensed form.

3.1
Properties

For most chemicals, the main physical properties are collected in public data banks and, while prediction models are available to estimate properties. Most companies have access to these data banks. Vapor liquid equilibrium (VLE) data have been assembled in the Dortmund data bank, while also safety properties have been collected in public data banks.

Problems arise when specific information such as kinetic models and kinetic constants and reactive chemical data are required. In general, reaction kinetics are considered to be company property unless they are published, or are for sale. Some engineering companies sell reactor models commercially, with or without their kinetic parameters. Another example is the kinetics of a crystallization step, though it must be stressed that these are disturbed considerably by the presence of impurities which require local measurement.

Reactive chemical data are not yet available in data banks though at present efforts are being made to develop such a data bank for pure components. An alternative way of collecting these data is through the suppliers of the chemicals, who will (by necessity) have knowledge of these properties. The reactive chemical data for the conditions in the process must be determined experimentally by the producer, in order to ensure a safe design and operation.

3.2 Modeling

Modeling is the heart of the quantitative understanding of processes, and this is reflected in the vision of the European Chemical industry, (CEFIC) (http://www.cefic.be under CAPRI (Competitive Advantage through Process Information Technology)), which is rephrased as follows:

- Process plants have models for design and operation to embody knowledge and understanding of the process and products, and to appreciate its underlying phenomena and behavior.
- The modeling environment and the models should be easy to program, robust, and with an open architecture to permit the exchange of data between models. The modeling environment (including its model library) must have direct access to a consistent set of supporting facilities such as: property data banks, economic evaluations and estimation sections, optimization routines, expert systems as adviser, external programs, and on-line data exchange to operation.
- The models should be organized as an integrated set of life cycle process models (Figure 3.1). They should facilitate the modeling from chemistry phenomena through unit models to process models, to be utilized for simulation, design optimization, control design, operational studies, and operation optimization, as well as business models. Product properties should be modeled up to and including end-product usage.
- The models should be able to run on readily available, standardized computing systems.

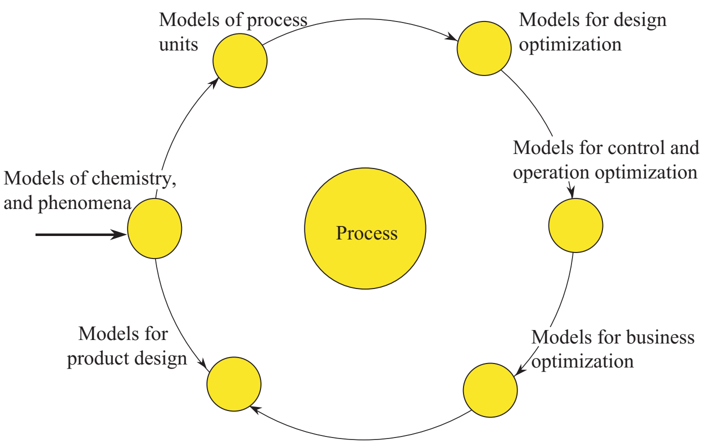

Fig. 3.1. Integrated set of life cycle process models.

The migration of the modeling tools in the proposed direction should, according to CEFIC, lead to excellence in:

- product innovation;
- improved and new unit operations and processes;
- enhanced interaction between chemistry, engineering, operation, business and product development, and
- optimized process operations.

3.2.1 Process Modeling is the Way to Improve Your Process

"Any model is better than no model". This ideal can be compared with the training program of a sportsman, who might suggest that "any training scheme is better than no scheme". For the design and economic operation of chemical processes within safe and environmentally sound constraints, models are essential. The above statements all reflect vision inclusively the vision of CEFIC that process knowledge resides in models, and we should realize that a complete range of modeling environments (simulators) and models are available commercially.

The following differentiation's may be made among models:

- Linear versus nonlinear models (LP versus NLP)
- Static versus dynamic models
- Sequential versus equation-based models
- Continuous versus mixed integer model environment for optimization (NLP versus MINLP and LP versus MILP)
- Unit models versus flowsheet models
- Empirical models versus fundamental models
- Design versus rating models
- Specific models such as:
- – molecular modeling
- – flow modeling/mixing
- – product property models as a function of reactor conditions, for example polymer properties
- – vent sizing packages
- – reliability modeling
- – dispersion modeling
- – quantitative risk analysis models

All these models have common aspects that require specific attention, with model *validation* being one of the most important. The constraints (and their applicability range) need to be known, and are often based on the basic assumptions and applicability of certain equations.

The *accuracy* requirements of the model might differ for each application. It is understandable that any inaccuracy of an operation optimization model results in a lost opportunity, and this will be discussed in **Chapter 9**. This in comparison with the accuracy of a dynamic model for control design, which does not require the same level of accuracy.

Generic process simulators (e.g., from Aspen Technology, Simulation Science, and Hyprotech) have physical property banks, unit models, economic sections and optimization routines available. The availability of cost estimation data is still limited, and is to be seen as a short-coming. Currently an estimating package is available which can be connected to the simulators, but at present it is very detailed, the initial approach being to use it for authorization estimates. This makes it far to detailed for use in process evaluations and optimization during conceptual design, where it is used on a comparison basis. The cost estimation section is a requirement to find the most optimal design. Another current short-coming is that, for optimization, the equipment costs should be described as a continuous function to avoid discontinuities.

The challenge is to *benefit consistently from process knowledge encapsulated in the different models*. Major software suppliers support this concept, and have as their objective the development of one modeling environment with a broad spectrum of models, as supported by the CEFIC vision.

3.3 Design Philosophies

The overall definition of the simple and robust process plant is:

1. An optimally designed safe and reliable plant that is operated hands-off under the most economical conditions; this is also called a "competitive process".
2. The ultimate objective of the chemical industry is to make long-term maximal profit; this objective emphasis two basic elements – maximize profit and long term.

3.3.1 Profit

The element of "profit" means that the industry must make a margin on capital. The element capital should be minimized in comparison to the margin that should be maximized. Historically, the trend was to maximize the margin through improvements on capacity, and raw material and energy utilization, with less emphasis on capital. In the design philosophies presented here, we address both aspects as equal partners.

3.3.2
Long Term

The element of "long term" emphasizes that we must have an ongoing, good relationship with customers and the community. Customers are satisfied by consistently low prices, good quality of products, and deliveries on time. Today, the communities represent moving targets, and the increasing standards of living of communities, together with the recognition that we must create a sustainable world for future generations, places a large responsibility on the shoulders of all civilians. In order to satisfy these moving targets we must do more than simply conform to changing local requirements. As a result of the increases in standards of living, the risk and nuisance requirements of communities become increasingly stringent, next to pollution loads, and a long-term vision with regard to environmental requirements is needed. The requirements include for example the ban on ozone-depleting gases, the CO_2 targets, and ongoing efforts to develop a sustainable world.

The ten design philosophies to be discussed must satisfy the ultimate objective of the competitive plant.

Design philosophies can be approached from three different perspectives:

1. Design of simple and robust chemical plants (Koolen, 1998);
2. World class manufacturing (Schonberger, 1986); and
3. Inherently safer and environmentally sound chemical processes.

The Design of Simple and Robust Chemical Plants

3.3.3
Minimize Equipment, Piping, and Instruments

The title of this philosophy may seem surprising, since it is unlikely that equipment that is not needed would be installed at all! The answer should be found in the way that engineers develop designs: they are accustomed to thinking and working in a sequential mode, and generally also have some fall-back (default) solutions at hand, some of which might include:

- When we need to transport a liquid, the fall-back design will be to select a pump and specify its type. Wrong! The first two questions to be asked should be:
  1. Do we *need* to transport the liquid? – and are there any alternatives?
  2. What will be the best way to transport the liquid? (Think about gravity flow, flow on pressure difference, before the default pump is selected.)
- When we need to move large quantities of materials, we design an inventory facility at the distribution point and at the receiving point. The first two questions to consider are:
  1. What will the most economical way? Do we *need* to move the material? – what might be the alternatives?

2. What will be the most economical way to transport it? Like mode of transportation, volume and frequency of shipment, this requires supply chain optimization

Note: In principle, one has to see the transport containment as a moving inventory.

On the subject of sequential thinking, consider the selection of a sequence of distillation columns. Let us assume that distillation has been selected on good grounds as the optimal separation technique, and that the engineer has studied and selected the optimal sequence of distillation separations, including energy optimization. The result is a sequence of subjacent distillation columns, but we still have to answer questions such as:

- Do we *need* to separate in a sequential way?
- Can't we combine the separation in a unit? (Think about separation of three or four components in one column either through the application of a simple side stream/stripper or with a divided wall column).
- Can't we apply a dephlegmator? (for details, see **Chapter 5**)

Another example can be seen in a sequence of distillation separations, where we may separate the first component A, followed by B and C. The overhead of the first column is condensed, collected in a reflux drum, and then pumped to the next column as a default design (see Figure 5.32 in **Chapter 5**). However, the solution might be *not* to condense the total overhead stream but only the reflux (avoiding the need for a reflux drum) and to accommodate the vapor feed to the next column (Figure 5.33 in **Chapter 5**). This situation is an example of what is called:

"do, undo, redo"
or "climbing a hill, descending the hill, and climbing it again".

In the above-mentioned, we brought a stream to a higher exergy level, decreased it to a lower level, and brought it back again at a higher exergy level. Typical situations to be avoided are: heating–cooling–reheating, pressurizing–depressurizing–pressur-

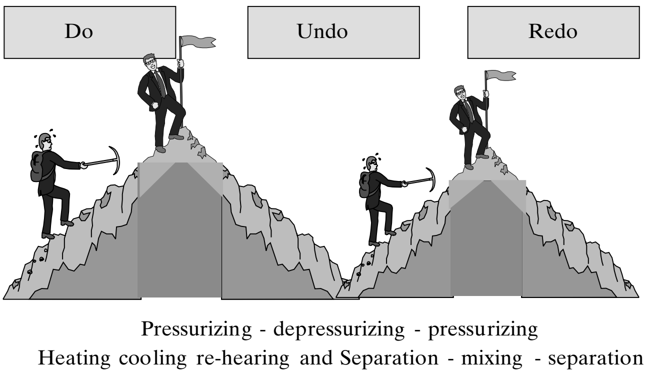

Fig. 3.2. Avoid a repetition of process steps.

izing, concentration–dilution–re-concentration, or separation–mixing–separation (Figure 3.2).

In the above examples it was the intention to illustrate that sequential thinking and default design approaches lead to conservative designs. The solution is to stimulate creative thinking, particularly during the conceptual design phase of a project.

Within a value engineering technique a methodology known as "function analysis" was first developed during the 1960s (Bytheway, 1965), and later described more extensively (Snodgrass and Kasi, 1986). This methodology (which will be described in more detail in **Chapter 10**) is based on setting up a brainstorming team to achieve simpler and more economical designs. After the initial design has been developed, the team is challenged to reduce/simplify the design. At that stage, the brainstorming often achieves limited results with marginal proposals. The reason is that the team members often have difficulties in achieving a sufficiently high level of abstraction to identify "out-of-the-box" ideas. *The methodology of function analysis creates a higher abstraction level, with help from a trained value engineer, by defining the basic function of the design steps.*

For a process plant design the index flowsheet is reviewed step by step on its principal functions. The function is described as an "active verb" and "a noun". The question is, does the step add value and if so, can the function be realized/improved by alternatives? All options to achieve the objective of lower cost with maintaining the ultimate objective to make long-term maximum profit are evaluated.

The most generic questions are:

- Do we need this process, unit, equipment, utility?
- Can we replace this functionality by an external service?
- Can we avoid this step by combining it with another step?
- Does it add value for the customer?

The brainstorm team lists the potential project alternatives and evaluates these in concert with the project team on added value for application, see **Chapter 10**, Appendix 2 for more details.

Minimization of piping and instruments should be addressed during the development of the P&IDs (process and instrument diagram) and the HAZOP (hazard and operability) studies. Historically, during P&ID development the addition of lines and instruments is a "sport", which is seldom lost by anyone who likes to add an item. All the items will form part of the final estimate, and from that perspective are not a burden for the project manager. There are mountains of rationales and arguments to justify the inclusion of an additional item. In general, a situation is pictured which will result in an unacceptable situation if it is not dealt with at this time. The likelihood of such an occurrence is often beyond discussion at this point, and the only way to solve the increasing levels of items during P&ID's development is through the participation of critical engineers, by questioning the inclusion of items, based on the following points:

- Why do you need this item?
- What would happen if we did not have the item?

- What is the likelihood of the pictured situation?
- Can we prevent this situation? (*"prevent versus cure"*) – bear in mind that any piping interconnection increases the level of complexity.
- Do we really need this for operation, or is it simply a nice addition for maintenance or design?
- What is the added value?

Simple and robust plants are often stripped of piping and instruments in order to make the system more surveyable and less vulnerable to operational errors and instrument failures. This places a high demand on the correct selection, location, installation, calibration, operation and maintenance of the instruments to achieve a high level of reliability and availability .

Summary

- The introduction of process simplification is handicapped by the way in which engineers think. The tendency is for them to think sequentially and in default solutions, while combinations or "out-of-the-box" solutions are seldom applied. The answer should be found by introducing brainstorming techniques, with a detailed functional analysis of the process.
- A process design often repeats process steps by doing, undoing, and redoing. A process stream is often brought at a higher exergy level, reduced in the next step, and increased in the following step. The challenge is to recognize these situations and to find solutions that avoid them.
- The keywords for simplification minimization of functions are:
– Eliminate/avoid
– Substitute
– Combine/integrate
– Added value?
- Minimizing piping and instrumentation makes the design more simple and surveyable, but requires a critical approach. Correct selection, installation and operation of these items is essential for reliable operation to be achieved.

3.3.4
Design of Single Reliable and Robust Components

The design of single reliable and robust components, unless justified economically or from a safety viewpoint, has a major impact on the low-cost design of process facilities. The investment of all spare installed equipment is under discussion, including the interconnections and any automatic stand-by provisions. Multiple process trains are also a target for cost reduction, and these are achievable if time is taken and effort applied to first recognize and then remove the technical barriers.

Historically, only very expensive equipment such as centrifugal compressors and turbines were installed as single pieces after maturation of the compressor/turbine technology. The result was that techniques were developed to improve the mechanical reliability of these units, including governors for speed control as well as improved bearings and seals.

Parallel to the development of more reliable machines was the trend to increase the capacity of single machines/equipment. Larger equipment could be manufactured to satisfy the demand from industry for the design of higher-capacity process plants, and thus increase the economy of scale. The need to keep these large-capacity plants operational was a major incentive to invest in reliability and robustness of all equipment. The increase of time between overhauls was another requirement from industry as a means of reducing cost and increasing the availability (up-time) of the plants.

The result was that techniques came available to increase the mechanical reliability and up times of facilities. For example, in the case of rotating equipment specific improvements were made in bearings, seals, and protective instrumentation, while the general design trends were to:

- design more reliable equipment;
- design larger equipment; and
- design for longer stand times, and higher availability.

For vessels, heat-exchangers, and fired equipment the increase in size and reliability were realized through improvements in:

- the selection of materials of construction;
- the mechanical design to reduce and cope with thermal and transient stresses;
- improved operation to reduce thermal and transient excursions;
- improved process design; and
- the prevention or reduction of fouling through chemical means, for example the use of inhibitors or the development of other catalyst systems.

The demand for larger process equipment was fulfilled not only through application of the above techniques, but also through the development of new mechanical designs. The constraints for larger equipment in general were the mechanical design and the fabrication capability. This not only forced the development of new equipment designs, it also forced the introduction of new process designs, including: (i) the scale-up of glass-lined jacket reactor vessels, which required alternative means of reactor cooling, such as feed cooling or the development of a reflux condenser; and (ii) the scale-up of styrene reactors, which changed from packed vertical-flow reactors with a tubular heated section to staged radial-flow reactors with interstage heating. Similar solutions were applied to other packed adiabatic reactors, such as ammonia reactors.

The reliable operation of in particular, smaller components/units ask specific attention. Generic components are available from several suppliers who service different markets. The development of these components pass a development cycle that is important to be recognized for application and selection in simple, robust plants.

The development cycle of components may be divided into generations:

- 1st generation products must improve on reliability due to initial short-comings.
- 2nd generation products improved on reliability, robustness, and implementation.
- 3rd generation products will be reduced in price, but there will be wide variation in the reliability of such components from different suppliers.

The lessons from the above with regard to generic components are to:

- hesitate before applying a 1st generation product in critical applications; and
- carefully select products from the 3rd generation, as their performance may be questionable – the reliability of the facility will also depend on these "common/generic" components.

The suppliers of assembled equipment such as cooling machines or compressor trains were forced to achieve high levels of reliability. Thus, it is vital for these suppliers to select, install, and calibrate the individual components and its instrumentation very carefully. These suppliers often have records of maintenance and failures which are available to support equipment selection detail.

The application of reliability modeling and the need for RAM (reliability, availability, maintainability) specifications for equipment will be discussed under reliability. The availability and understanding of reliability techniques and tools is a prerequisite to introduce the philosophy, "design for single reliable components unless ...".

The improvements made in reliability and availability of components, and the capability to apply reliability modeling, make that philosophy a reality which brings considerable savings in cost and capital. However, be aware that in line with simple design we may say:

There is no component more reliable than no component

Summary

- The mechanical reliability and robustness of components/units has been improved considerably, this having been driven by the market.
- The economical size of equipment and process units and processing trains have been increased considerably. The increase in sizes became achievable through improved mechanical designs, modified process design, and larger fabrication facilities.
- The reliability and availability of a process is also determined by the fouling of process equipment and catalyst systems, and this requires the close attention of R&D investigations.
- Selection of small or assembled equipment require specific attention from a reliability perspective
- Reliability techniques are available to evaluate design alternatives.

- All critical equipment from a reliability perspective need to be ordered with a RAM specification next to its duty specification.
- The single component philosophy is achievable, and brings about high reductions in both cost and capital.

3.3.5 Optimize Design

Until now, the optimization of process design has been the result of evolution, as engineers have been stimulated to improve their designs through external circumstances. Examples of this include the energy crisis, increasing environmental requirements, product quality requirements, and market competition. More recently, the increasing focus to achieve a sustainable world has been added to this list. A good illustration is the process flowsheets of a batch process at different stages of development (see **Chapter 1**, Figures 1.4–1.7).

The evolution of a process plant is clearly illustrated in that example. The evolution of plant designs will continue, particularly in the field of reactor technology based on the design of catalysts. The demands on environmental requirements will become even more severe, the emphasis coming from the drive for a sustainable world – in other words, higher selectivities and lower utility consumption will be foremost. In future, communities will need to be convinced by industry of the application of sustainable technology. The global market conditions will put pressure on low cost, resulting in further optimization of the design and its operation, and this in turn will lead to higher levels of integration between processes.

Although for new designs, careful evaluation of available designs and the evaluation of process synthesis options will become major requirements, the application of the current process synthesis tools are limited by:

- The tools are not yet sufficiently mature.
- The data required as input are of limited availability, notably for the evaluation of different reaction/separation techniques.
- Limited applicability to existing situations – bear in mind that most plants have lifetimes of 30–40 years and are subject to major modification every 10 years.
- Industry is not willing to take large risks related to new technology/designs (conservatism).

Optimization of the design will provide considerable improvements in efficiency (Douglas, 1988; Biegler et al., 1997; Koolen et al., 1999; Seider et al., 1999). In industry, the current practice of optimization is restricted to a comparison of selected cases by the engineers; this situation must change, and is supported by ongoing research in this field.

Research to solve the conceptual design as one discrete optimization problem will advance, and indeed the modeling environment is evolving in that direction. The conceptual design of a process plant will ultimately not be solved as one problem, on the basis that:

- The alternatives for the design will still be subject to the inventiveness of the designer. There is no doubt that the quality of the synthesis tools including generation of design alternatives will improve, but (as learns the examples for simplification in **Chapter 5**), there is still a long way to go.
- Designers always want to keep track of the decisive steps in an optimization effort. They tend to follow a step-wise approach, with intermediate validation of results and reconsideration of active constraints.
- Optimization software is currently not sufficiently robust to solve major optimization problems, nor to include the effects of integration and controllability.
- Designers will (in agreement with business) always try to minimize the risk of a design, and therefore often take a more conservative route. This does not mean they do not *want* to quantify the best design – but they may decide on another route.

Based on the above conclusion, process synthesis have to be carried out at different hierarchical levels. The detailed levels that are discussed follow an interactive onion model, which is based on the conventional onion model of Smith and Linnhoff, 1988.

Between these different hierarchical levels, interaction and process simplification need to take place in order to optimize the total plant design, as is illustrated in Figure 3.3.

The optimization will be done in a layered approach. It starts with the evaluation of many process alternatives. The number of alternatives will gradually be reduced while the modeling details will enlarge. Ultimately one overall process flowsheet

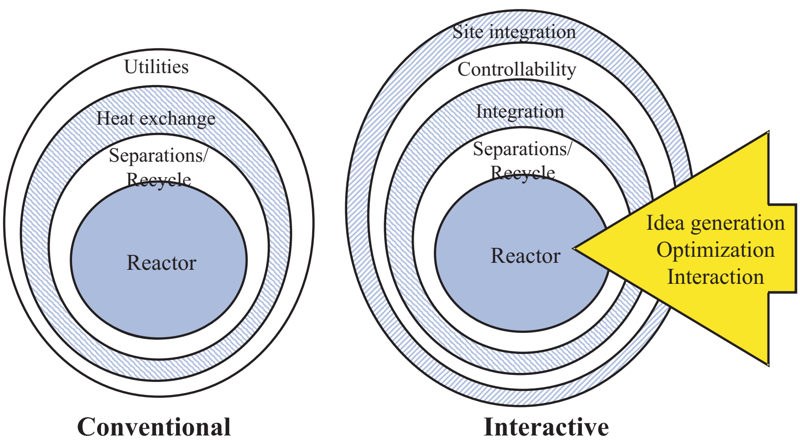

Fig. 3.3. The interactive onion model versus the conventional onion model.

will be selected for the simultaneous optimization of process conditions and equipment dimensions, see **Chapter 4**.

This methodology has as advantage that all decision steps can be followed and intermediately validated while active constraints might be reconsidered.

Process simulation with a sufficiently detailed reactor model, with options for mixed integer problems including cost estimation and economic sections, are a requirement for design optimizations.

Summary

- Design optimization will increasingly be applied; the driving force for this increased emphasis will be – next to economic consideration – the need to comply with a sustainable world.
- A layered optimization approach will be followed by the engineer to maintain an insight in all decision steps during the design process. Ultimately, an overall optimization model will be used to optimize design of the selected overall flowsheet.
- The simulation environment needs to be mixed integer, and equipped with estimation and economic sections to handle the design as a single optimization problem.

3.3.6
Clever Process Integration

Process integration is a development that is inherent to the trend of further design optimization. All types of integration within between– as well as between – processes will be studied in order to optimize the design. Next to heat integration, power, cooling, refrigeration, water and hydrogen integration are also studied to achieve better overall performance.

In general, the integration studies are performed under steady-state conditions, without any consideration for either the dynamic effect or the availability of the streams. As such, the integration might be seen as a contradiction to process simplification because it makes the design more complicated. Referring to the formulation of complexity in **Chapter 2**, it is clear that this will add to the complexity. Integration will have its effect on complexity, as the following terms will be increased: the number of equipment pieces, interconnections, input and output DI&DOs and AI&AOs, but particularly the disturbances will increase – and this as such may introduce interaction.

There are two ways to reduce complexity:

1. By application of a higher automation level.
2. By de-coupling the system to achieve robust control.

The previously mentioned examples of a complicated piece of equipment such as a TV set or a household refrigerator are simple to use due to their high level of automation. However, de-coupling must be carried out in terms of both hardware and software wise.

Process integration can be differentiated as follows:

- Direct integration between process units with process streams.
- Integration between process units on "utilities" levels, such as energy and water.
- Integration with utility plants, for example in plant power generation.

Hardware de-coupling is illustrated in Figure 4.28. A direct cross-heat exchanger between two process sections can be de-coupled by installing two additional heat exchangers – a back-up heater, and a cooler. Integration between units at utility levels is shown by replacing the process cross-heat exchanger by two exchangers with a utility steam back-up. The hardware de-coupling mainly tackles the availability.

For integration within the same process section direct exchange is often applied. Integration between process sections of the same plant is quite frequently done by exchange at plant utility level. Integration between different processes is preferably done through exchange at site utility level.

Software de-coupling is illustrated in Figure 4.29. In this example of a distillation column, the heat produced from an external source passes to an exchanger that is operated in parallel with an existing steam reboiler that can take the full load. By measuring the total heat duty of the exchangers and manipulating that heat duty for control purposes, the systems are de-coupled and compensation is made for external disturbances. A similar solution can be applied to the source side. In this way, it is possible to cope with the availability as well as the disturbances.

The problem of availability and vulnerability is a major issue for a chemical complex, particularly if the level of integration is increasing (Koolen et al., 1999). Optimization of the design of an integrated chemical complex with regard to availability and unit/service reliability will be discussed in **Chapter 7**.

Summary

- Process integration is increasing at all levels, with progressive pressure to improve performance in terms of raw materials and energy utilization.
- Process integration may conflict with simple and robust plants, and must be addressed by a higher level of automation and control.
- The major concerns of process integration are availability and disturbances.
- Back-up provisions are often used to cope with availability during outage or malfunction of integrated units. In general, integration between processes is carried out at site utility levels in order to provide back-up.
- Disturbances are rejected through the introduction of advanced control techniques.

Optimization of the design and operation of chemical complexes needs to include an availability study based on the reliability of the units/services.

3.3.7 Minimize Human Intervention

Human beings are both highly creative and intelligent – characteristics which make it possible to improve our way of life. Another characteristic is that humans are always prepared to learn on a trial-and-error basis, in addition to receiving education. Consequently, whatever is learned there is always the desire to confirm such learnings. Another human characteristic is its difficulty in repeating things in consistent manner; thus an airline pilot will conscientiously follow a checklist before start-up, and this is cross-checked by the co-pilot.

Human beings are not consistent in performing tasks, and so it is necessary to protect process systems for mishaps during operation of a process plant. The philosophy to minimize human intervention is translated as:

design for total automation and robust hands-off control

of a chemical plant, and in this respect the operator will change to a supervisor with limited operational tasks.

The advantages of this approach may be considerable:

- Man-power savings: it might be possible to use only one operator for two mid-sized, continuous plants.
- Improved control, resulting in less off-specification products.
- Higher-capacity operation through the application of constraint controllers on feed streams.
- Less maintenance due to mechanical failures as a result of operational errors or uncontrolled stops/transients.
- Operation optimization, with its own savings, can be introduced on top of the robust control layer.

3.3.7.1 Total automation

At present, the tools for total automation are available, and current instrumentation systems have this capability. The automation strategies must be transparent and may differ between plants, but this isn't preferable if they are planned to be operated by one person.

An automation strategy must emphasize the following elements:

Level of automation: in an automated plant not all operations are automated. In most cases it is preferable to provide a minimum of operation attention in a supervisory role. To enable this, certain process actions must be fulfilled by an operator to keep him actively involved in the operation.

- Level of process checking: in batch processes, reactor loads of different components are often checked with a double independent measurement based on a different measuring principle. This is in agreement with Total Quality Control.

- Process sequences for start-up and shut down with detailed step descriptions.
- Alarming strategy including interlocking and trip actions.
- Protection levels – who has access to what.
- Program testing.
- Operator training on sequences and interrupts.

3.3.7.2 **Robust hands-off control**

In the present situation a panel operator is still part of the control loop, but this situation needs to be resolved. It is not an easy task, and will require additional investment in the design of robust control. The control of a process is carried out in three hierarchical layers, see Figure 8.2:

1. Basic control: this must be designed in such a way that it functions independently of the model-based control, as well as the operation optimization layer.
2. Model-based control: this will be dependent on the basic control layer, but can operate independently of the operation optimization layer.
3. Operation optimization: this layer depends on the basic control layer, as well as the model-based control layer.

Basic control design is currently mainly based on heuristic rules (Luyben et al., 1998), the governing philosophy of which is: "*It is always best to utilize the simplest control system that will achieve the desired objective*". In respect of the hierarchical control layers (of which the model-based and optimization layers cannot be considered simple), a philosophy for the basic control layer is introduced in line with Luyben's statement:

Basic control design has conceptual to be simple

This concept means that we should avoid closing loops which will cause much interaction, but will also avoid inverse responses. These situations would require intense operator attention and thus would not comply with a simple and robust design. For example, if an operating unit has two controlled variables and two manipulated variables that cause a high level of interaction (e.g., the two qualities of a distillation column), it is preferable to close only one quality loop. In practice, the stream used for internal recycling will not be directly quality controlled, and this stream will absorb the disturbances. In the case where both streams are final products, one stream will run at a higher purity if the model-based controller is not functioning. In the case where the interaction or disturbances can be de-coupled at the basic control level by simple algebraic equations, it should be implemented at the basic level.

The design of basic control configuration will move from heuristic to fundamental design procedures, whereupon the following aspects must be considered:

- Control design will have to be carried out in interaction with the process design. Controllability analysis techniques would be used to select the final flowsheet to balance optimal design and controllability.

- Control design will be based on fundamental control strategy design for the selection of the best loop pairing, to maximize disturbance rejection and minimize interactions, in particular to facilitate operation at the basic control level if the higher levels of hierarchy are not operable.
- Optimal control loop design is performed based on dynamic simulations, and incorporates the selection of instruments and its location in process, valve selection and sizing, vessel dimensions and controller design.

The design of the best pairing of control loops can be performed by making use of controllability parameters such as the relative gain array to show the steady-state interaction, and dynamic parameters (e.g., disturbance condition numbers) (Seider et al., 1999 and control text books).

3.3.7.3 **Model-based control**

Model-based control (MBC) is also known as model-predictive control, as it may anticipate predicted conditions (Skogestad and Postlethwaite, 1996). The present advanced technique for the development of robust, model-based controllers is based on input/output models which are developed based on a model identification technique. However, the current development of these controllers has the following disadvantages:

- They are designed after the plant has begun to operate.
- They are linear, with a limited operating window.
- The development of an input/output model is time-consuming, and must be repeated after each process modification or where there are unidentified operation conditions, for example another feed composition.
- The development of input/output models is inaccurate due to the limited availability of process measurements.

In future, model-based controllers will also be designed, based on fundamental dynamic models. The development of these will be less time-consuming as they will be derived from static (equation-based) models, as part of the life-cycle models. In the near future, it is likely that model based controllers will become nonlinear and applicable in a much larger operating window.

The objective will be to automate operation and achieve robust hands-off control in order to minimize operator intervention, though plant "trips" will occur more often compared with keeping a plant on-flight with minor operator adjustments. As a result of this higher level of automation, operators will acquire much less hands-on experience, and will be trained using dynamic plant simulation models. Basic operator training will focus on plant behavior, and basic response on upsets. The operator will be trained in situations where the MBC is out of operation, and only basic control is functional.

Summary

- Human beings possess characteristics that make them less capable consistently to execute the same tasks.

- Total automation and robust hands-off control can overcome these handicaps, and will result in considerable savings.
- A common automation strategy needs to be applied for different process plants operated by the same personnel.
- Control design for basic control as well as model-based control will be based on fundamental dynamic models, while nonlinear controllers will find applications.
- The training of operators will need to be adapted to concur with their new role.

3.3.8
Operation Optimization Makes Money

Operation optimization is a broad area where considerable savings can be achieved. The optimization might be split into business models and process operational models, but as both types have a similar basis they will each be mentioned in the following section.

The business models include:

- Planning models for products; this is particularly important for batch plants and continuous plants with campaign operation.
- Supply chain optimization applied to product distribution over several customers.
- Feedstock evaluation; this is particularly important for plants that handle different feed stocks, for example refineries and ethylene plants.
- Overall operational models (as used for refinery complexes) to optimize a chain of plants.

The process optimization models referred to include:

- Scheduling for batch and campaign operations
- Scheduling of equipment in relation to batch operations
- Optimization for continuous processes based on actual feedstock, product, and utility prices. The optimization emphasizes the selection of:
- – optimal process conditions
- – optimal capacity (if not set by the business)
- Optimization of dynamic operations as batch and transient operations regarding operational and capacity conditions. Optimization of the run times of fouling systems will be carried out in combination with the operational conditions, e.g., catalyst aging or coke formation.

The optimization models for businesses are based mainly on linear programming (LP) techniques, which are faster to develop and execute. The businesses need to explore many options – hence the need for a rapid response. In addition, feedstock evaluators and overall operational models need to be highly accurate, and are therefore derived from the more accurate process optimization models.

The process optimization models (with the exception of planning models) are in general based on non linear programming (NLP) techniques and are equation-based. Most process plants have a strong nonlinear behavior, while at the same time the profit margins are only a few percent of the operational costs. These factors require the models to be highly accurate, and to be validated over their operational range.

A "profit meter" designed as an envelope over the total process plant is an excellent tool for use in overall model validation (Krist et al., 1994). The profit meter can also be used as an instrument to obtain and evaluate real-time plant performance data for production, as well as for business people to maximize profit by varying process conditions.

The technology for dynamic and continuous optimization is relative new, but is maturing. Savings realized through optimization are considerable, but are differentiated by type and by application. Savings for each type of optimization are of the order of magnitude 2–4% of operational costs, and may be $\geq$10% if savings on constrained controllers and capacity utilization are included. The impact on actual profit might be of the order 10–20%, or even higher, depending on the profit margin.

Summary

- Operation optimization can be split into business and plant optimization applications.
- Business optimizations are applied to planning, supply chain, feedstock evaluations, and overall business operation.
- Process optimizations are applied to scheduling, operational conditions selection, and transient operations.
- Process optimization models need to be highly accurate as the effect is in the order of a few percent of operational costs.
- Profit meters are designed to measure plant performance in real time; they are used for overall model validation and evaluation of plant performance by operation and business.
- Operation optimization may make a significant contribution to profit margins.

World-class Manufacturing Perspective

3.3.9 Just-in-Time Production (JIP)

"Just-in-time production" is a term that was introduced in the 1970s and 1980s, and was part of the quality wave which started in Japan. In particular, JIP came from the car industry, where the logistic costs are extremely high, but since then it has found its way through all industries. The principle is that a product is produced at quality (total quality control) when isit is needed, the objective being to reduce the logistic costs. The same applies for feed streams which are to be received, which one might call "just-in-time receiving".

A striking example is the paint industry where, in order to reduce the number of color compounds for distribution to the final customer, base colors and color concentrates are sent to the shops. When the customer arrives in the shop the required color composition is prepared while he or she waits for their request to be carried out.

In the process industry, several techniques are applied to implement the JIP concept. In batch or campaign plants, only basic products are stored to a limited extent. The additives for each customer are added either during loading into the transport truck/system.
container/railcar, or at the customer's location, using a local dosing system. Loading of material might be through a revolving manifold, and be automatically operated, in order to minimize piping at the loading station. The ultimate option is to load the product from the process directly into a transport container, without any storage (see Figure 1.7 in **Chapter 1**).

Minimization of storage and operational cost is the main challenge of the supply chain. Optimization should be carried out with respect to the transportation cargo size, frequency and reliability of supply, processing reliabilities, storage volumes and the customer delivery requirements, (Figure 3.4). The delivery requirements are a trade-off between storage capacities transportation cost and the probability of capacity loss, due to unavailability of product. The methodology for optimization of storage is based on probabilistic inputs of processing and transportation deliveries and Monte Carlo simulations. The technique is known, and will be discussed in **Chapter 7** (Storage optimization). The ultimate aim of JIP is to have a line between two production facilities, without any storage. This may sound optimistic, but in the case of gaseous feeds that is often a standard solution, especially in cases where materials are highly toxic or flammable (e.g., chlorine, HCl, H_2, CO), and also for natural gas and hydrocarbons such as ethylene and propylene. The transport of liquids through pipelines to processes in the neighborhood is being used increasingly.

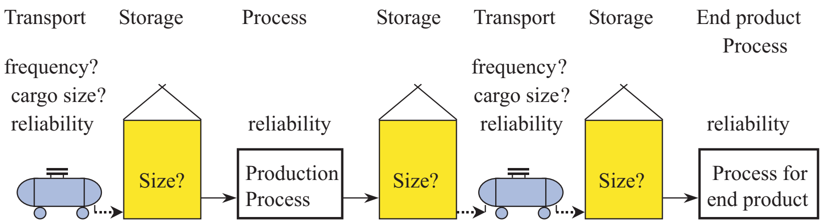

Fig. 3.4. Optimization of a supply chain based on reliability and availability data from transportation, production process, customer processes.

Summary

- JIP is a concept to minimize storage, and is based on quality production and supply chain optimization.
- JIP aims to minimize the stored products to base components, and supply additives during loading or at the customer's location.
- Design of storage capacity at the plants and at the customer's location is based on processing reliability, transportation frequency cargo size and reliability, and customer delivery requirements.
- The methodology is available for the optimization of design and operation based on Monte Carlo simulations.

3.3.10 Design for Total Quality Control (TQC)

3.3.10.1 Prevent versus cure

The concept of JIP can only be applied if we are able consistently to produce at specification.

Elimination of check and lot tanks Prevent versus cure, which is part of TQC, makes it attractive to eliminate corrective provisions such as the check tanks and lot tanks in plants. These tanks are installed in plant recycle systems to cope with off-specification products.

In the past, most batch plants were unable to produce consistent batches, and therefore more batches were produced and the whole was blended in a so called lot tank The solution for this is to use feed forward control (in general to be double-checked with separate measurements) with a feedback adjustment in the process. The disturbances (whether internal or external) should be incorporated in the feed forward controllers to achieve TQC (see Figure 1.3 in **Chapter 1**). It should not be underestimated that operational errors are also often a cause for off-specification situations, and these must be covered by the application of automation.

Prevent upsets Many provisions are installed in plants to cope with unplanned situations. The release of a component to the environment is mostly covered with add-on provisions such as scrubbers, incinerators, flares, emergency tanks, etc. However, all of these provisions are expensive, and the best way to handle the situation is to modify the design into a preventive action, triggered by a question such as:

what provision is needed to prevent an upset?

A higher design pressure of a vessel in order to prevent release, or release through a safety device into another process vessel, are often cheap solutions. The following is a typical example (Figure 3.5). The safety provisions on an ammonia storage facility asked for a very large scrubber with water, and the recovery of unlikely, but potentially diluted, solution. Removal of the safety device was accomplished by preventing upsets. In this particular situation, a potential fire was the limiting case. Elimination of the potential for fire by installing a sprinkler system on the tank, and the removal of any adjacent fire source formed part of the solution. Additional solutions included the elimination of all other potential pressure increases by installing instrumental protection with appropriate precautions and in-process relief.

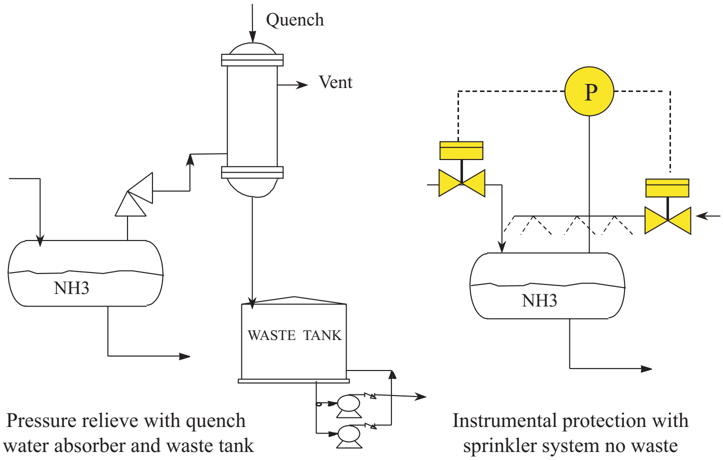

Fig. 3.5. NH_3 storage with recovery system versus a simple instrumental protection system.

3.3.10.2 Design for first-pass prime production

The design of first-pass prime (Aelion and Powers, 1991; Verwijs et al., 1995) is a concept that has not yet been extensively explored, though it has the same objective as "prevent versus cure". The concept is to avoid expensive provisions in plants in order to cope with off-specification products that have originated from the start or recovery of a facility. A careful design of start-up and standby procedures is required to achieve the objective of first-pass prime production, see **Chapter 8**. Therefore, it is important to distinguish between process units as being reversible or irreversible.

A *reversible* unit operation is defined (Verwijs et al., 1995) as: "A process system that can be operated stand alone without any process stream fed in or out of the system, due to the presence of inverse operations". This yields the possibility of conditioning a process system during an operational state of the process. Irreversible unit operations can only be operated by supplying an appropriate feed.

Automated plants have defined process states. Next to the actual production state, transient steps are defined for start-up, shutdown, and product changes. Process wait states, also called standby, are also introduced, which have defined process conditions, before the process is moved to another operational state. Process wait states can be differentiated in:

- Cold process wait condition (cold standby): at this state the inventory in the units is established.

- Hot process wait condition (hot standby): at this state the inventory and defined temperatures are established.
- Recycle process wait: at this condition the inventory, temperature, pressure, specifications and internal recycle streams are established.

The cold process wait is the cold starting condition for an initial processing step.

Hot process wait or hot stand-by is a condition which forms the bases for actual production at temperature. Examples include a steam turbine which is at slow roll with a slipstream of steam to enable fast start-up, or a distillation column at total reflux.

Recycle process wait can be applied to reversible unit operation where all process conditions, including an internal recycle, are established. Examples include an evaporator where the bottom and overhead stream are returned as recycle, a distillation column with recycle of its top and bottom stream into the feed, or a refrigeration unit with a minimum cooling duty from a reversible process unit.

The development of the hot stand-by and recycle mode condition as a start for the production is essential in order to achieve first-pass prime production. Most plants have a reaction section followed by a finishing section. In such a configuration it is a standard approach to have the downstream finishing section in such a condition (hot stand-by or recycle mode) that the process and products are at specification before any feed is started. For irreversible units, such as a reactor or an extraction, a recycle mode cannot be established. In these situations the system must be pre-conditioned to such a level, to produce on-specification products from the start. For a reaction section, a hot stand-by condition is often established by recycling one of the components or a carrier over the system at the required inlet temperature. Such a pre-selected condition in line with a hot stand-by or recycle finishing section will enable smooth start-up and first-pass prime for production. It should be said that sufficient effort needs to be spend in analyzing the system dynamically to develop such an operational procedure. In all cases, a thorough understanding of the process (often reflected in a dynamic simulation of the process) is required to meet this objective.

Summary

- Just-in-time production (JIP) has as objective to minimize the logistic provisions. It requires production on request and at specification, following the concept of total quality control (TQC).
- "Prevent versus cure" is an approach to prevent off-specification production, resulting in the elimination of intermediate storage and blending facilities for products out of specification. Implementation is often realized through feed forward control actions and direct recycle provisions in the process.
- Production of first-pass prime product requires an operational strategy to avoid plant provisions for recovery of off-specification products.
- The development of operating strategies with intermediate standby conditions leading to the first-pass prime production are essential. The development of operation strategy requires detailed process knowledge to be captured in dynamic models.

Inherently Safer and Environmentally Sound Perspectives

3.3.11
Inherently Safer Design

The development of inherently safer chemical plants is an objective that was introduced by Kletz (1991) and later extended further and promoted by the Center for Chemical Process Safety (CCPS, 1996) from AIChE and IchemE. The basic concept was covered in four guiding words:

1. Minimize
2. Substitute
3. Moderate
4. Simplify

Before the meanings of these words are described in detail, the following example will serve as an illustration. A storage tank is planned for a rather nasty, liquid material (product "X") which has the following qualitative properties: a low boiling point; decomposition which starts around boiling point; solidification which occurs some degrees below the boiling point; high toxicity; flammability; degradation with oxygen; and exothermic reaction with water.

Let us consider an overview of the safety provisions that would need to be installed on such a storage tank.

Safety provisions are:

- Measurements resulting in signals/actions on high and high-high, low and low-low signals on level, pressure, temperature, oxygen detector, water detector.
- Pressure protection PVRV (pressure valve and relieve valve), ERV (emergency relieve valve), inert padding, flame arrestor.
- Safe let-down systems for vapors.
- Protection against tank leakage.
- Inhibiting system.
- Insulation.
- Indirect heating to avoid high tank skin temperatures.
- Loading and unloading requires seal-less pumps with dead-heading and temperature protection, excess flow protection, vapor return lines.
- External protection such as fire detector, toxicity measurement, sprinklers, water-guns, fire brigade at stand-by, emergency plan for the site and the community, quantitative risk analysis (QRA) available, dispersion calculation information available on-line.

All the above provisions are add-ons, and accept the situation as it was submitted (Figure 3.6). Although the above is an extreme example, the point to be made is applicable to storage of chemicals – that protection is with add-ons.

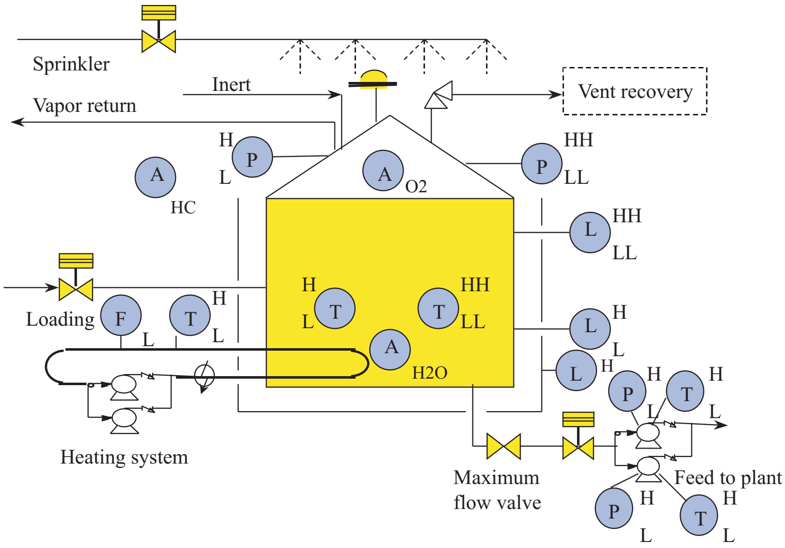

Fig. 3.6. Safety provisions of a storage tank for product X.

Some basic questions for storage tank designs from an inherently safer design perspective based on the four guiding words are:

Minimize

- Do we really need the tank? Could product X be supplied by pipeline?
- Can we avoid storage and handling by direct feeding from process to process?
- Did we consider feeding to the process in the gas phase (less inventory of toxic material)?
- Did we consider a smaller tank?
- Did we consider buying in containers to avoid handling and feed on pressure into the process?

Substitute

- Do we really need this chemical?
- Could we replace it with a less harmful product?

Consider the effects of vapor pressure, toxicity, flammability, reactivity, inter-reactivity with other plant components, solidification point, product degradation. All these properties add to the safety provisions.

Moderate

- Do we really need the chemical in the form as it is?
- Can it be handled in a less harmful form? For example in dilute solution, another phase, mixing with another inert material. You might consider low-

ering vapor pressure, reactive chemical properties, flammability limits, lowering solidification point, sensitivity to other plant components.

- Could it be supplied with another (essential) material that we need so that handling can be minimized and conditions moderated?

Simplify

- No tank.
- Do we need the process feed pump? (Options are gravity flow, or transport under pressure difference)
- Did we consider seal-less pumps?
- Could we load under pressure difference instead of by pumping into the tank?

A typical practical example which came to my attention was a tank with caustic soda used as a neutralizing agent for a waste water facility. The tank was equipped with a set of metering pumps, which were adjusted by a pH controller. The metering pump required a lot of operation attention and maintenance due to fouling. One day an accident happened when an operator was sprayed with caustic soda and injured, despite his wearing protective clothing. The incident resulted in a root cause analysis of the system, the four major questions of which were:

1. Minimization: Do we need caustic storage?
2. Substitute: Can we use another neutralizing agent or can we prevent neutralization?
3. Moderate: Do we need the high concentration?
4. Simplify: Do we really need to pump?

Different solutions were studied, but the final choice was to: (i) decrease the caustic concentration to meter larger flows with a standard flow meter and feed at gravity flow; and (ii) remove the pumps – to achieve this the tank need to be elevated only 1 m. The new design was much safer, simpler, and more robust (Figure 3.7).

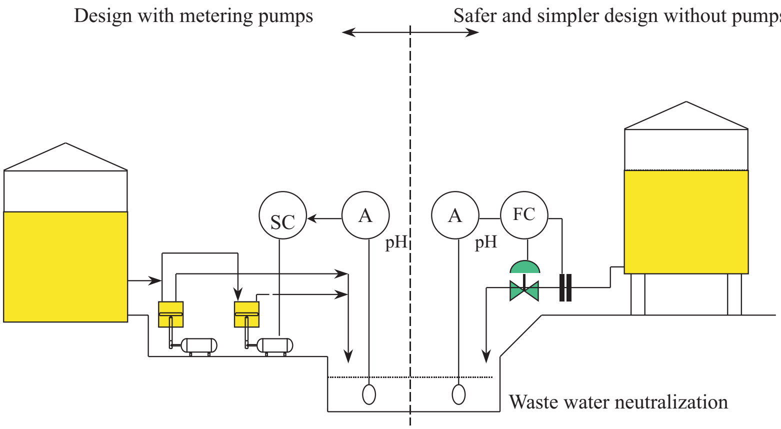

Fig. 3.7. Dosing with metering pumps versus gravity flow.

The above illustration emphasizes the benefit of evaluating inherently safer design philosophies during the design. As a standard, safety reviews are performed during different stages of the design of a process, and often result in add-ons. The evaluation of the inherently safer set-up during the conceptual design forms the largest contribution to simple robust and safer design. (For a reference to this, see the excellent training package of the IChemE on Inherently Safer Process Design.)

Summary

The application of inherently safer design philosophies based on the guiding words: “minimize”; “substitute”; “moderate”; and “simplify” result in a safer design and in a more simple and robust plant design.

3.3.12
Environmentally Sound Design

While environmentally sound designs might be seen as a local problem, it is the author’s opinion that such an approach may lead to designs with high cost over the lifetime of a process. Environmental requirements are subject to rapid changes; initially, these were driven by the western world but are becoming increasingly global as they are also adopted by developing countries.

Both the designs and the products must comply with a minimal environmental load. During the last decades of the 20th century all types of technical solutions were developed in order to minimize the environmental load. Inevitably, such developments will keep pace with the environmental requirements.

The concept of sustainability is introduced at global scale, driven mainly by the United Nations (see ISO 14040/41/42/43). This is defined as: “*sustainable development meets needs of the present, without compromising the ability of the future generations to meet their own needs*” (Brundtland, 1987).

The development in sustainability is one which is also strongly influenced by consumer markets. An example is the car industry, which analyzes the environmental contribution of individual components selected for the production of cars that are more environmentally friendly. Similar results have been published in Eco-profiles of the European plastic industry (APME, 1997).

Next to the pollution of air, water, and soil, the main environmental factors of concern are those of nuisance and risk. Nuisances,- such as noise and skyline pollution-, driven by local situations, will in time, evolve to generate more stringent local requirements. Risk of processing facilities and transportation of hazardous materials will have to comply with more stringent governmental regulations.

Consequently, processes designs will need to attack environmental problems by using a sequential approach (Figure 3.8):

- Prevent/minimize
- Recycle in process/reuse in process
- Recycle between processes
- Destroy with recovery

- Destroy without recovery
- Controlled waste disposal (to be avoided, but like in the mining industry it isn't avoidable)

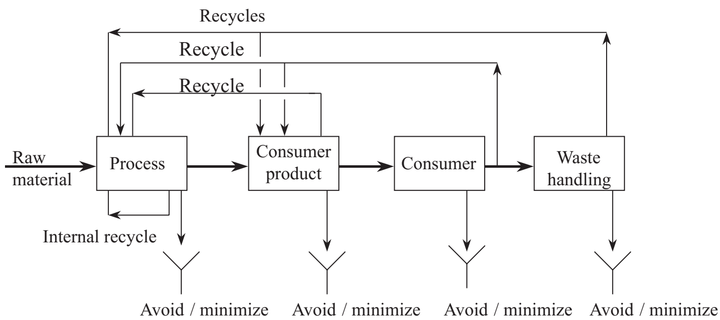

Fig. 3.8. Environmental levels of attack, minimize losses, recycle internal and external, destroy with recovery and without recovery.

The technology of process integration, and increased recycle and reuse of material, leads to more selective operations. Environmentally sound designs ask for detailed process knowledge and simulations to predict the impact of potential build-up and removal of recycle components. The integration of processes asks for clever solutions and correct hardware and software de-coupling of systems to enable robust operation.

The level of complexity is increasing through these design requirements, but in order to comply with simple design requirements the level of automation and robustness of the control must be addressed next to the application of simple design techniques.

Summary

- Environmental requirements will strengthen and will be increasingly globally driven.
- Sustainable product developments will have a long-term impact on product design, as well as process design.
- Nuisance requirements will be local in nature while risk criteria for processing facilities and transportation will be set by governmental regulations
- Detailed process knowledge and simulations are needed to predict the impact of build-up and removal of recycle components.
- Environmental requirements may lead to more complex designs that need to be neutralized by a higher level of automation and control next to the application of simple design techniques.

3.4 Design Philosophies are an Integrated Set

The above ten design and operational philosophies are to be seen as an integrated set of philosophies. The impact and integration as an example of the evolution of the batch plant is illustrated in **Chapter 1** (Figures 1.4–1.7). By comparing the different generations of plant with the final design, the following application of philosophies can be identified:

- Inherently safer design
- – Avoidance of opening of equipment
- – Elimination of hydrocarbon hydro carbon (HC) storage by direct feed to avoid inventory of hazardous material
- – Elimination of HC mix tanks by in-line mixing to avoid problems of reactive chemicals and storage of hazardous materials.
- Environmentally sound
- – Vent recovery.
- – Elimination of HC storage prevents loading and breathing losses.
- – Less product storage prevents product leakage.
- – Less handling of additives prevents spills.
- Minimize equipment
- – Elimination of HC storage tanks by direct feed.
- – Elimination of HC mix tanks by in-line mixing.
- – Replacement of additive tanks with dedicated containers.
- – Avoidance of more reactor trains by development of large reactor system.
- – Avoidance of lot tanks by improved feed forward control.
- – Elimination of final product tanks evolved through basic product storage in storage containers.
- – Elimination of post reactor and devolatilization vessel by finishing in the reactor.
- – Elimination of product cooler by cooling in reactor vessel.
- – Vent condenser included in overhead condenser.
- Design for single reliable components
- – Single reactor train.
- – Pumps to be single, not shown on the flowsheet.
- Optimize design
- – Application of design philosophies as single component, minimize equipment, etc.
- Clever process integration
- – Integration of supplier plant by direct feed of HCs.
- Minimize human intervention
- – Minimization of batch time by automation.
- – Improved feed forward control to improve product consistency to avoid lot tanks.

- Operation optimization
  - Capacity constraint controller on feed.
- Just in time production
  - Direct HC feeds, resulting in removal of HC feed tanks.
  - Elimination of product storage.
- Design for total quality control
  - Automation of plant to obtain consistent production.
  - Elimination of lot tanks by improved feed forward control for consistent product

The design philosophies represent an integrated effort and all take part in an overall activity to obtain,

> *an optimal designed safe and reliable plant, operated hands-off at the most economical conditions.*

It should be mentioned that these philosophies can also be applied as stand-alone philosophies, especially in an existing process. In **Chapter 10**, which refers to the operation and continuous improvement of a quality plant, special attention is given to the improvement of existing facilities – which often form the basis for the design of a new facility. Some aspects should be mentioned at this point. Hands-off operation can be developed for an existing process by tabulating what operators are doing; a plan may then be developed to minimize theses activities by ongoing screening. A similar situation exists for maintenance, as well as for just-in-time production, whereby the operation is run at minimum stock so that storage is made available for other applications. In addition, it is folly to install and maintain a spare compressor when it could be removed and the operational unit made more reliable.

The ultimate savings for the design or upgrading of a process based on the design philosophies are very large. In practice, a capital saving of 30–40% on capital cost can be achieved, while savings on operational cost are in the order of 5–10%, depending on the plant. Savings on maintenance should reduce in equivalence to the capital reduction, but also be less than 1% of invested capital. The number of operational personnel will also be reduced, their activities shifting from operation to supervision, and focusing on low-cost operation.

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Chapter 4
Process Synthesis and Design Optimization

Process synthesis and design optimization is the most important part of a design. It determines the efficiency and the economics of the process plant. Nevertheless the importance of this activity there wasn't an structural approach developed over the years up to the last decades. The approach taken so far was based on an evolutionary process. Step by step the processes were improved hand in hand with opportunities which were identified and developed at research. The objective of process synthesis and design optimization is to systematically evaluate design alternatives to derive at the optimal process. In this chapter a step wise methodology is described how to derive at an optimal designed process.

The conceptual process design to achieve high-quality processes is a layered approach based on the conventional "onion" model as discussed by IChemE (1982) and by Smith and Linnhoff (1988), see Figure 3.3. A more detailed hierarchical approach to conceptual design was published in the trendsetting book, *Conceptual Design of Chemical Processes* (Douglas, 1988). Hierarchical, layered approaches have been discussed in great detail more recently Douglas and Stephanopoulos, 1995, Biegler et al., 1997; Seider et al., 1999). The conceptual design developed along the layers, from inside to outside in the onion model was presented in the following sequential order:

- reactor
- separation and recycle system
- heat exchanger network
- utilities

In this chapter the onion model will be broadened with integration (a wider term than heat exchange network), controllability and site integration (a much broader field than utilities).

The layers in the adapted onion model are:

- reactor
- separation and recycle system
- integration
- controllability
- site integration

The onion model is complemented with an arrow crossing all layers to emphasize the need to interactively design between the different layers, while applying optimization techniques and simplification efforts through idea generation as tools to evolve to the optimum process design. The modified onion model is named the interactive onion model to emphasize the interaction between the layers in comparison to the conventional onion model, Figure 3.3. Process interaction optimization and simplification between the layers will form a "red line" through this chapter.

The onion approach seems contradictory to those who like to solve all the options as one large structural optimization problem, in a MINLP (mixed integer non linear program) environment. It is the author's opinion that this will not happen during the approaching decades because:

1. The number of design options that may be implemented is greatly underassessed; in other words, there is an incomplete set of design options. Options often evolve *during* a design – they are not available beforehand. Some examples of process simplification illustrating the impact on the development of a distillation sequence are shown in **Chapter 5** (Section 5.3.2). There is no doubt that in the long term, process knowledge and design alternatives will be extended and captured using a structural method.
2. The problem structure often leads to non-convex optimization problems, which in turn usually leads to locally optimal solutions (or not).
3. Engineers always wish to keep track of flowsheet development in order to understand and evaluate the choices. In other words, even if the process design can be captured and solved as one problem, engineers will evaluate the steps in the program in a layered manner so that they understand the logic and bases behind the crucial decisions.
4. The mathematical techniques available are not (yet) sufficient to cope with these large-scale MINLP problems

Based on the above arguments, the hierarchical approach is preferred where design decisions made at each level of hierarchy bound the optimal solutions, which was also concluded by Douglas and Stephanopoulos 1995.

The strong point is that a synthesis methodology, computational tools and search algorithms exist to evaluate and optimize the search for an optimal design. The weak point in the whole synthesis process as by to day is the lack of a structured set of design alternatives. The design of a process still heavily depend on the creativity and experience field of the process designers to develop alternative options. The development of heuristic rules for the pre-selection of alternative separation units made progress but the disadvantage will remain its inherent restricted validity and applicability. The development of a separation system is next to the reactor section the most challenging tasks. It is here where Douglas and Stephanopoulos 1995 made progress by introduction of the general separation system superstructure, see Section 4.2.2 on separation.

4.1 Process Synthesis

Process synthesis is the activity which sets the economics for the process for at least the first part (if not longer) of its lifetime. Most process design improvements occurred as the result of an evolutionary process, and in general a process is adapted on three or four occasions during its lifetime in order to update it with respect to the actual economic market and recent developments in technology.

In this chapter we concentrate on the development process, but advantage will also be taken of developments in synthesis tools. The latter topic is currently undergoing a particularly rapid development cycle: consider the high availability of modeling tools that are available as static and dynamic simulations and optimizations for process design, control design, and operation optimization. Despite the emphasis that academia is placing on the development of the synthesis tools in the short term, their contribution to industry will be limited, for the following reasons:

- The number of new designs is limited, as in general a process is retrofitted several times during its lifetime. During such retrofits the degrees of freedom (DOF) are limited due to hardware and logistic situations that current synthesis tools are incapable of handling. Currently, development exist to address retrofit pinch analysis techniques for heat integration (Asante and Zhu, 1996; Briones and Kokossis, 1996).
- The risk of design modifications for new designs that are acceptable from a management perspective is limited. Businesses take risks with new designs, and this can lead to losses over a period of months. In reality, improvements are introduced in step-wise fashion. Licensors who build similar processes have a better change for these gradual improvements, but they are also limited from a guarantee perspective.
- Grass-root process designs ultimately have many DOF, but these are also restricted. The physical and kinetic data required for these designs often are of very limited availability and need to be measured at laboratory scale. Moreover, they also require extensive verification if they are outside current operational experience, in order to minimize the risk.

The advantages of process synthesis techniques will be – next to development of grass root designs – its application as instrument for process analysis and the identification for opportunities. They will show the direction in which process research and developments should proceed. The requirements for sustainable technology development are also setting opportunities which will drive for wider application of synthesis tools.

4.1.1
The Hierarchical Structure for Conceptual Design

The hierarchical structure for the conceptual design process is an extension of the structures proposed earlier by (Douglas, 1988; Smith and Linnhoff, 1988; Douglas and Stephanopoulos, 1995; Biegler et al., 1997; Seider et al., 1999).

The approach to the synthesis of a process is based on the interactive onion model and presented for a known technology area. This is a quite common situation in industry, the scope of the project being set by the business based on the market situation. It includes projected capacity, product slate, product qualities, and technology selection. A technology selection is the first technological step in a project, the selection being a combined effort between business, R&D, and process technologists. The technology selection is based on technology that is available – either commercially or within the company. During technology selection, decisions concerning the basic process route and the batch-versus-continuous process question are taken in agreement with the business (for details, see **Chapter 10**). The starting situation for a process synthesis study is, in addition to selection of the technology, the outlining of a feasible flowsheet, together with reaction and reactor information in a modeling format that has been developed during the research phase. Both types of information are very useful during the first approach of the process synthesis. Although these initial designs are not optimized, they do generate some initial data for conversion and recycling costs for unconverted reactants, as well as capital costs. These data can be used for the initial reactor evaluations, which will be updated as soon as the separation train has been synthesized.

The hierarchical structure has the following layers:

1. Reaction, selection of configuration.
2. Separation, selection of types and sequence.
3. Integration, types and level of integration.
4. Controllability analysis, static, dynamic.
5. Flowsheet optimization, of sections and the overall process.
6. Logistics and site integration.

The conventional approach of process synthesis is pictured in Figure 4.1.A, which shows a sequential design while the interaction between the different layers is shown as reverse directed dashed arrows. The hierarchical approach developed and presented in this chapter is shown in Figure 4.1.B, with a more detailed presentation is presented in Table 4.1. This concept differs in; the introduction of a two overall development steps, which are separated by an idea generation step. The different layers shown in two sequential overall steps indicate the gradual development and interaction between the different synthesis layers. The interaction shown between the layers within the same step is indicated by dashed lines while the overall flow line is shown as a solid line.

Idea generation is shown as a separate activity between the overall steps in order to emphasize the importance, and the best place for implementation. The idea generation particular addresses the introduction of process simplification techniques

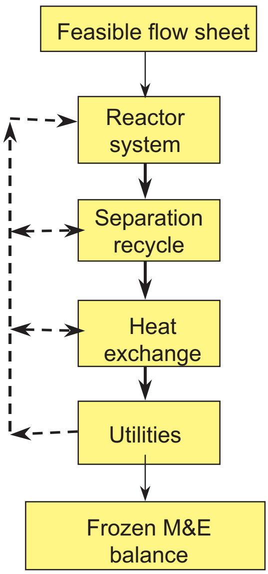


Fig. 4.1-A. Conventional process synthesis methodology.

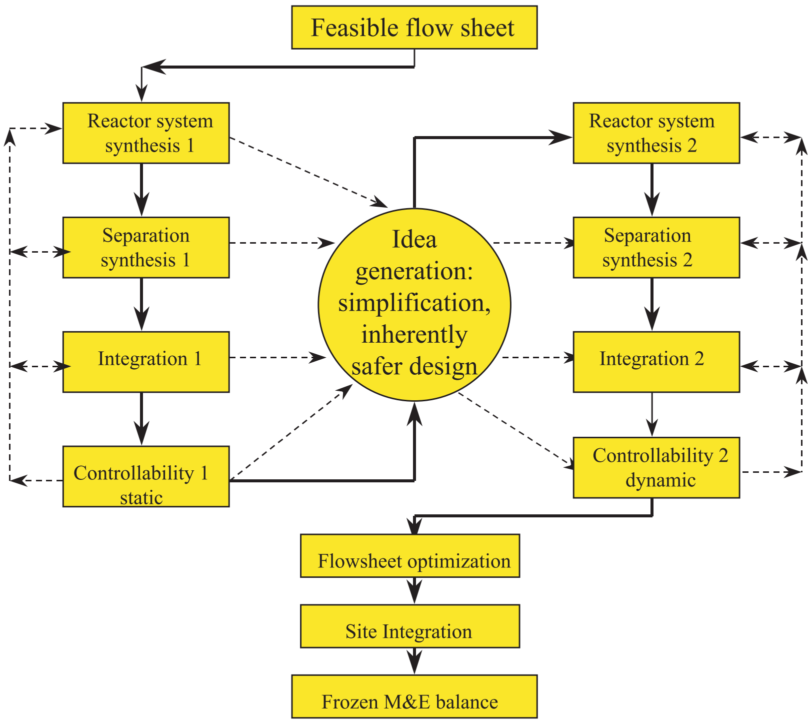
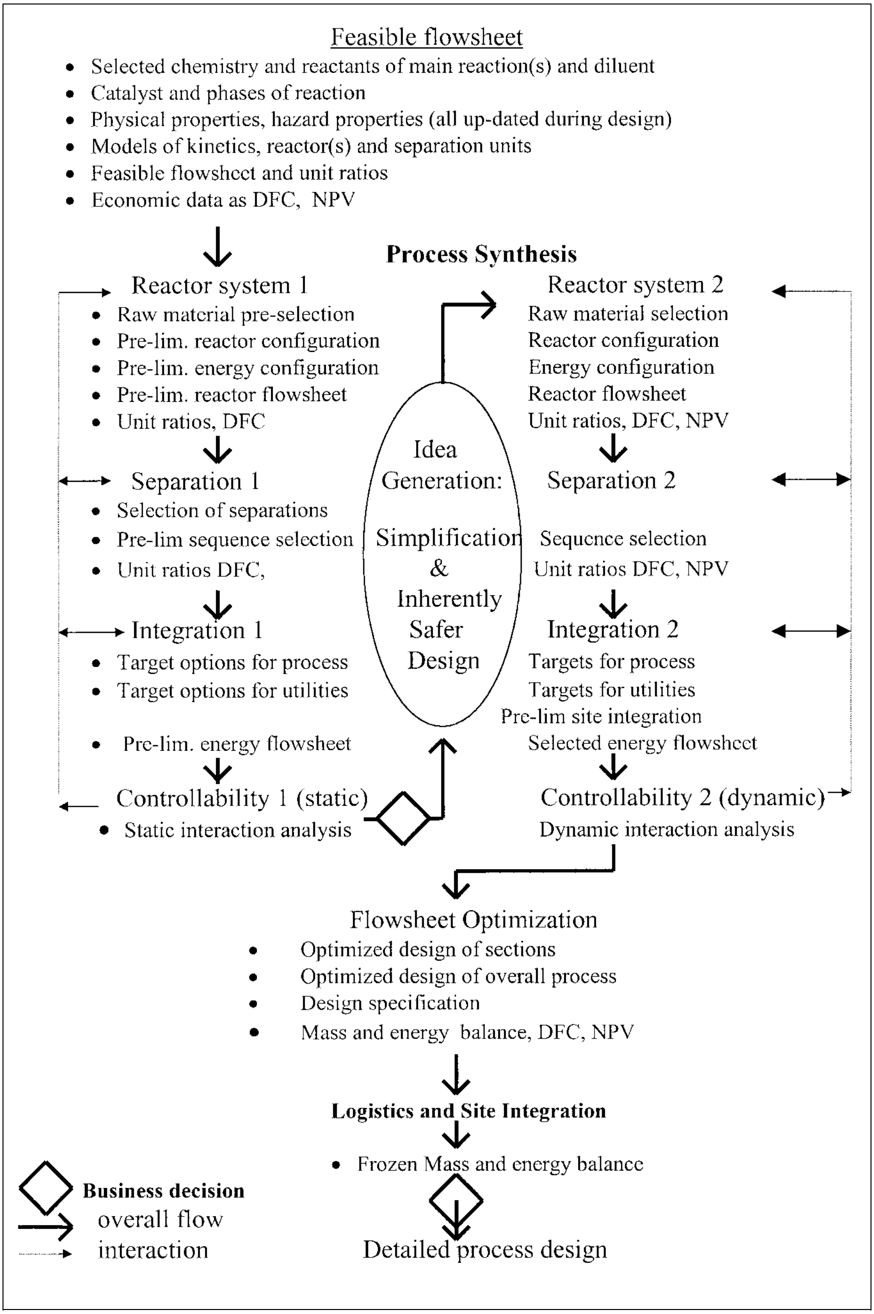


Fig. 4.1-B. Step wise process synthesis: methodology.

Table 4.1. Conceptual design flow diagram with deliverables and interaction, (NPV net present value, DFC direct fixed capital).



inherently safer design techniques. The concept is based on the assumption that designers are not capable to generate all potential solutions right at the start of a project. Designers will remain creative and generate new alternatives during the design process and therefor an essential part of the proposed methodology is to include a place for evaluation and reconsideration of alternatives. Simplification and inherently safer design are an important part of the idea generation next to identification of alternative units and configurations.

The fact that the layers are shown in a sequential order illustrates the decision-making process. In reality, there will be many parallel developments to speed-up the conceptual design, including:

- Selection of separation technique in step 1 will take place parallel to reactor development in step 1.
- Controllability 2 will take place parallel with the other development in step 2; the time-consuming step for development of dynamic models would otherwise delay the progress.
- The parallel effort is justified, although the final conclusions about controllability 2 can only be drawn after integration and equipment in preliminary sizing are finished and controllability analysis is finished.

It was said before that next to idea generation and interaction, optimization was an essential part of the synthesis process. The optimization effort is performed at each layer and step, while the interaction between the layers is reflected in the economic values for the intermediate streams which as such will have an impact on the composition of the intermediate streams. Interaction between reaction, separation and integration should converge to an overall optimized design. The optimization is approached in four layers which are over laying the synthesis hierarchy and is shown in Figure 4.4 The optimization will start with the evaluation of lots of alternatives and shrink gradually to one final flowsheet where process conditions and equipment dimensions are simultaneously optimized. The optimization methodology be will discussed in more details in the Sections 4.1.4 and 4.1.5.

Controllability is split into static step1 and dynamic step 2 as early feed back to the designer about any controllability problem is essential.

Flowsheet optimization is seen as a separate layer, an activity after the synthesis has been completed and stream compositions and equipment dimension are tuned to a final optimal flowsheet.

Logistics and site integration are the complementing activities to achieve an optimal integrated process at the site.

The overall activities in the layers – there is no split made between the activities in the two separate steps – are described as follows:

- Reaction
- – Evaluate chemistry and raw materials, reactants purity
- – Evaluate potential hazardous/toxicity of chemicals storage and handling
- – Evaluate reactor types and conditions, the excess of reactants and the options to shift the equilibrium

– Apply process simplification
– Select reactor configuration and raw materials
– Select reactor conversion and selectivity
• Separation
– Collect physical, chemical, hazardous/toxicity properties, and equilibrium data for relevant phase separations, of all involved components
– Develop an input and output process stream diagram, and identify all input and output impurities by thoroughly detailed analysis of the reactor's inlet and outlet, as well as any degradation product of additives as inhibitors
– Evaluate potential separations
– Select separations
– Apply process simplification
– Evaluate sequence of separations and select two to three flowsheets for integration studies
• Process integration
– Evaluate major options for integration within defined constraints (see next paragraph)
– Apply exergy and pinch analysis technique to minimize targets for utility consumption and integration opportunities
– Evaluate preliminary site integration alternative
– Apply process simplification
• Controllability analysis – static
– Steady-state analysis for controllability and resilience (C&R) for flowsheet alternatives
• Controllability analysis – dynamic
– Determine dynamic C&R analysis
• Process flowsheet optimization
– Select the best flowsheet for optimization
– Divide process in sections and determine intermediate values and incremental values for recycle streams
– Optimize section by section
– Optimize overall flowsheet
• Logistics and site integration

The process synthesis methodology has been completed with two business decision points, see Table 4.1. It is important to include these activities in the development process as they have updated design input and ultimately require recent economics next to there business input to support a stop or go decision.

The approach for a process synthesis methodology practical for industry is summarized as:

- Selection of a starting point of the synthesis being the evaluation of existing process technology resulting in a preliminary selected feasible flowsheet.
- Development of a hierarchical structural (layered) methodology based on the interactive onion model.

- Application of interactions between the different development layers; break with the doctrine of solving problems sequentially.
- Reduction of the size of the synthesis problem by dividing the process into sections for optimization (see Sections 4.1.4 and 4.1.5).
- Inclusion of idea generation as a place for reconsideration of the design and implementation of process simplification and inherently safer design techniques in the methodology.

Further details on the methodology for process synthesis are discussed in the following sections, while the potential options for simplification are discussed within the different synthesis layers.

4.1.2 Constraints to Process Synthesis

Constraints play an important part in the synthesis process, and must be recognized in advance if unnecessary work is to be avoided. Typical constraints include:

- Availability of physical and chemical properties
- Safety
- Environmental
- Decomposition reactions
- Fouling constraints
- Corrosion constraints
- Utility constraints
- Controllability (to be discussed under the controllability layer)
- Patents
- Product specification (most products have more specifications)

4.1.2.1 Physical and chemical property data

These represent a severe constraint for process synthesis studies. In order to achieve an optimal design, the intention is to evaluate several feasible flowsheets. Although some physical properties such as vapor–liquid equilibrium can be reasonably well predicted for most other units, the prediction of such properties is much more difficult and requires laboratory investigations to be performed. The availability of these data considerably limits the number of options for evaluation. However, this handicap of the process synthesis is still valuable, not only by identifying these shortcomings but also to increase the number of design options, which can be considerable.

4.1.2.2 Safety

Safety decisions during process synthesis have long-term consequences for the process and its logistic situation. These decisions must be taken not only for the reaction section and the main reactants, but also for all other chemicals used in the process. Raw material, (intermediate) product storage and transportation should also be included.

The design philosophies of inherently safer design and environmentally sound processes set the stage for these decisions (Kletz, 1991; CCPS, 1993, 1996 and a specific developed training package of IChemE, 1995). The risk of an operating facility and its surrounding areas must also be subjected to an extended evaluation as part of the synthesis study. Hazardous indices such as the Fire and Explosion Index (F&EI) and the Chemical Exposure Index (CEI) are useful as screening tools. In case of indices which are considered too high, measures might be taken by the elimination of chemicals or reducing inventory and hazardous conditions. The most important Safety Health Environmental (SHE) activities are to be planned during the initial synthesis layers, reaction, and separation. At this stage, the emphasis is on the prevention of hazardous situation, but later during the design the safety of the installation will be increased by add-on provisions, although this will address inherent safety aspects only to a limited extent.

4.1.2.3 **Chemical reactivity**

This requires special attention (CCPS, 1995), since it is the properties of chemical reactivity which set constraints on the design and operation of a facility. Identification of the hazards of chemical materials, mixtures and reaction masses is required. The reaction involved include not only decomposition reactions but also polymerization reactions.

The *thermal stability* of a component can be determined experimentally or theoretically, although on a theoretical basis the kinetic rates cannot be determined. A database is available which provides this information (Bretherick, 1990). The most frequently used software is called CHETAH, which screens organic, organo-metallic chemicals, inorganic salts and mixtures for their potential to undergo decomposition. This program is also very useful for the estimation of thermodynamic data such as enthalpy, entropy, heat capacity, and the Gibbs' free energy for specified reactions. The CHETAH program classifies the energy hazard potential of a composition by a pattern recognition interpretation based on several criteria.

The most common thermal and reactivity measurements are DSC/DTA (differential scanning calorimetry/differential thermal analyzer), these test methods being used as a screening tool. An advanced, commercially available method to obtain reactive chemical data is the accelerating rate calorimeter (ARC) (Townsend, 1981; Kohlbrandt, 1987). The ARC measures heat of decomposition, onset temperature, the heat rate as function of temperature, overall reaction kinetics and the pressure as function of temperature. It is an excellent tool for determining the design and operational constraints of a facility, and the data are also used for the sizing of relief devices. The ARC is – next for pure components – used to test all types of mixtures, and eventually can include solids such as catalyst particles, which might have an impact on the decomposition rate. The selection of the mixtures is based on the local compositions of the different processing streams.

Incompatibility of substances is another reactivity factor that plays a role in selection of the constraints of a process design. Incompatibility can be screened using DTA/DSC, but may also be identified using CHETAH. Advanced testing methods are known as reactivity testing and flammability testing. It should be noted that

these properties must be determined for all chemicals involved in the process. This includes the reactants and products, as well as solvents, any solid materials such as ion exchangers or adsorbers, catalysts, and utilities (water, air, nitrogen, oxygen, heating and cooling media) and construction materials, including insulation and gaskets. Be aware that the process also covers cleaning activities; thus, it is required that substances used during cleaning, washing and regeneration (e.g., solvents, regeneration materials, water) be included.
The reactivity properties must be documented, and the constraints for the design determined. For example:

- Do not heat exchange two substances which are classified as incompatible, as the heat exchangers might leak.
- Operate outside an explosion range.
- Avoid materials of construction in sections which might lead into a compatibility problem with process streams.
- Pyrophoric materials are not a preferable choice.

Mechanical sensitivity testing is divided into sensitivity to mechanical shock, and friction. These mechanical sensitivity conditions are to be avoided, and may lead to the constraint of a design. On occasion, the sublimation of shock-sensitive solids might be the cause of a major accident.

4.1.2.4 **Environmental requirements**

These have a growing impact on the design of processes, and are subject to moving targets as Society places more emphasis on this aspect over time, with strongly evolving global directions. The emission of pollutants will have to be absolutely minimized. The requirements will not be limited to steady-state conditions, and more emphasis will be placed on occasional situations. The drive for sustainable technology will enforce the industry to select more efficient routes from a sustainability perspective (Graedel and Allenby, 1995). Eco-profiles (APME, 1997) will be required, and standards such as ISO14040/43 will have to be applied to these studies. The sustainability studies must be performed during the technology selection stage of a process, but the results achieved in the process synthesis need to confirm these data. Sustainability is improved either by the selection of a more efficient route, or by process efficiency through integration between processes.

Add-on techniques to comply with emission requirements are generally available, but are still subject to improvements. The challenge is to *prevent* these emissions rather than to apply techniques of abatement.

An approach by which environmental losses may be attacked is illustrated in Figure 3.8 of **Chapter 3**, the sequential actions being to:

- Prevent/minimize
- Recycle in process/reuse in process
- Recycle between processes
- Destroy with recovery

- Destroy without recovery
- Controlled waste disposal (to be avoided, but like in the mining industry it isn't avoidable)

Process designs often apply internal recycling as a practical solution. There are often unrecognized constraints to recycling, and the build-up of impurities in recycle streams might lead to considerable problems. During process synthesis the separations are often designed based on the main components, while impurities are supposed to leave the process via vents, tar or product streams. The real answer must be quantified by determining all impurities in the feed and the reactor outlet. A mass balance which includes all impurities must be prepared, together with a clear identification of where they leave the process and where accumulation takes place. The installation of drag streams might be unavoidable. These impurities can become the key components for separations, and can have a major impact on the optimal process train.

4.1.2.5 **Decomposition reactions**

These may play an important role; if they are exothermal they are already considered under reactive chemical constraints. Product degradation without heat release can lead to an undesired situation for product purity and reasons of selectivity. They may also place constraints on the processing temperatures.

4.1.2.6 **Other constraints**

Fouling constraints might be reactive chemical constraints with very low reaction rates; they are very difficult to predict without long-duration testing. The effects are often experienced during operations such as reboiler fouling where the wall temperature might have an effect . Catalyst deactivation or aging are often measured in the laboratory or in the production plant, and can often be reduced by selecting other operational conditions. The root causes may be physical, and include the precipitation of solids as a result of temperature and concentration effects. The fouling of seawater exchangers, air compressors, and air coolers is subject to external sources. As the latter can be overcome by specific actions, they are – strictly speaking – not constraints.

Corrosion constraints may determine part of the separation sequence. The removal of highly corrosive material often leads to a need for very expensive and specific constructions. Consequently, such components are removed early in the process. An example is the nitration reaction which is processed in glass-lined or tantalum equipment, and where neutralization of these streams before further processing is standard practice.

Utility constraints in theory do not exist, as any utility level can be generated in the process, though in practice this might lead to high cost. Problems associated with low temperature cooling, or a need for temperatures above available steam temperature, can be solved but require high levels of investment – making the process less attractive.

Before a synthesis study is commenced, an inventory of the constraints must be made; moreover, extensive testing may also be needed in order to avoid surprises at a later date. Although the constraints on a process synthesis study are considerable, it is possible that by recognizing such constraints, engineers are sufficiently intelligent to devise clever solutions during process synthesis.

Summary

- Constraints have a major impact on the degrees of freedom for a process synthesis study. These constraints can be subdivided as: physical and chemical properties, safety, environmental decomposition, fouling, corrosion, utility and controllability.
- The hazards of a components or mixture and its incompatibility as present in the process must be collected, documented, and subjected to evaluation.
- The hazards of these components need to be used as input for the application of the inherently safer design principles during the first layers of the process synthesis and to define the constraints of the design and operation.
- Environmental requirements can be divided into emission minimization and sustainability. Both are subject to moving targets set by Society, but are increasingly directed by global concerns and regulations.
- Sustainability is a criteria for the selection of the process, and will impact on the development of new process routes. Sustainability also drives for higher process efficiencies that, next to improvements in process synthesis, also lead to further integration between processes.
- Emission minimization should preferably be achieved by more selective reactor/separation designs, eventually followed by efficient abatement techniques.
- Internal recycling is applied to aim at lower emissions. This leads to build-up of impurity levels, which demand a careful design of the separation system to achieve an optimal process. A mass balance covering all impurities, including formation, build-up and removal, is required for a good design.
- Decomposition reactions and fouling often place constraints on the processing temperature, but the wall temperature might also play an important role. Recognition of these constraints is important in order to avoid excessive cost in operation.
- Corrosion problems and utility restrictions are not necessarily constraints, but in practice they often exert a high economic penalty on certain synthesis options.

4.1.3
How Broad is a Synthesis Study?

A synthesis study is often started during and/or after the execution of a R&D project aimed at improving an existing process. These developments were triggered by an idea to improve a reactor system by developing an alternative catalyst system or reactor configuration. They focus on improvements of selectivity's and/or conversion, and examples include: conversion from gas phase to liquid phase reactions; improved catalyst systems; combinations of reaction; and separation such as a zeolite membrane reactor or reactive distillation. New reactor configurations, such as: switching from packed bed to fluidized bed system (Dutta and Gualy, 1999) or a homogeneous system, reverse-flow reactor systems (van de Beld and Westerterp, 1996); interstage component removal (Westerterp et al., 1989); development of a bubble column reactors (Schluter et al., 1992) are all improvements that have been explored. The results of this research are configured in reactor models. Improvements in separation are also often subject to detailed research activities. On examining developments at the grass-roots level it should be mentioned that these also focus on a particular catalyst system and configuration. The results of such research activity are included in what is called "feasible flowsheet models". Before the conceptual design with its synthesis study of a project is started, the results of research will be evaluated in the context of other process routes in a feasibility study.

The alternative options for the sequencing of separations will remain, but many processes have a limited number of separations, or have constraints which limit freedom with regard to the number of options available.

The limitations in technical knowledge and the constraints justifies the conclusion that improvements to an existing system or a grass-roots design often have limited practical alternatives to be introduced into a (preferably fundamental) model. The number of alternatives is also restricted due too the application of the layered approach- if this approach isn't applied the number would increase tremendously, this is at best be reflected in a decision Figure 4.5. The limited number of alternatives, and the ease of their simulation and overall design, makes the comparison of alternatives on a direct, economic basis and the avoidance of large optimization problems an attractive proposition. This does not mean that broad studies are not carried out. Indeed, one benefit of a broad study is the identification of opportunities for further developments. In the context of sustainability, a search for cheaper routes by increasing knowledge and solving constraints will undoubtedly gather interest.

4.1.4
Economic Calculations

Economics ultimately determine whether a process will be executed, and a number of factors play an important role in achieving an objective, optimal design:

- An economic evaluator and a professional cost estimator should be involved in the design team to ensure objectivity in the cost estimates and evaluations
- The cost estimator is responsible for updating estimation data for the specific location in the database used for the evaluation and optimization of process design alternatives as part of the simulator. Discontinuities in the cost data set for equipment must be smoothed in order to avoid converging problems during optimization.

- The economic evaluator must agree to the economic calculation set and the price sets to be used for the evaluation (price sets are ultimately determined by the business).
- The economics must be based on the net present value (NPV) of the project over its lifetime. Ultimately, the project needs to meet the criteria for NPV/investment. Any incremental investment to optimize the facility should meet these criteria set by the business. Hence, trade-offs between incremental capital and savings need to meet those economic criteria.
- The price sets used for evaluation need to cover a range. Experience teaches that price sets are subject to large variations over the lifetime of the process plant.
- The optimization results are strongly affected by the variation of price sets (one reason why operation optimization is applied).

Both design optimization and process synthesis are performed in process sections in order to obtain a better insight of the different DOFs for the optimization (Koolen et al., 1999). Thus, a process is split into sections and subsections. The methodology to calculate the intermediate prices is described below. The process taken as an example is the production of 1-octene from crude C4; this is described in EUR. Patent 0 461 222 B1 and EUR. Patent 0 561 779 B1.

The main reaction steps are:

$2\ C_4H_6 + CH_3OH \xrightarrow{\text{Pd catalyst}} C_8H_{13}CH_3O$
(exothermic liquid phase, homogeneous system)

butadiene + methanol $\rightarrow$ 1-methoxy 2.7.octadiene (MOD-1) (telomerization)
unwanted by-product isomer(MOD-3)

$C_8H_{13}CH_3O + 2H_2 \xrightarrow{\text{Pd catalyst}} C_8H_{17}OCH_3$ (exothermic gas/liquid phase)

methoxy-octadiene (MOD-1) + hydrogen $\rightarrow$ methoxy-octane ether (MOE) (hydrogenation)

$C_8H_{17}OCH_3 \xrightarrow{\text{Alumina catalyst}} C_8H_{16} + CH_3OH$
(endothermic gas phase, fixed bed)

methoxy-octane ether (MOE) $\rightarrow$1-octene + methanol (ether cleavage).

The overall process consists of three reaction steps followed by separation sections (see Figure 4.2). The bottom section of this figure illustrates the eventual split in subsections.

For the optimization and synthesis of the sections, the direct fixed capital (DFC) and NPV of the overall process are first calculated based on the raw material and product prices as supplied by the business and the available unit ratios. Based on the DFCs of the different sections, the NPV of each section is determined by splitting the overall NPV in ratio to the split in DFC.

The intermediate prices (prices between the sections) can now be back-calculated, starting from the last section forward, to comply with the NPV of the section. In the

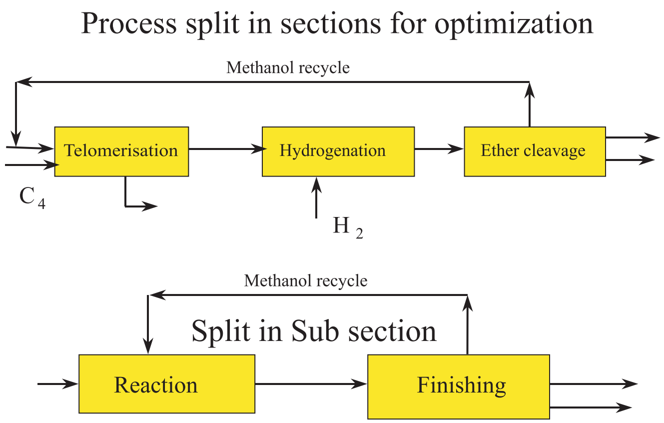


Fig. 4.2. Process split-up into sections and subsections for optimization.

example there are two methanol recycles which are valued differently. The recycle from the last section back to the first section is valued at market value, while the recycle from the separation section of the first section is valued at incremental cost and capital for this specific stream to be spend in the separation section. In this last case the methanol conversion is low, and the value is used to optimize the conversion of methanol.

These intermediate process streams are updated each time that more accurate information becomes available from the sections.

At the beginning of the synthesis study data are used from the feasibility study. After this, the data are updated intermediately based on the selected flowsheet and updated DFCs.

4.1.5
Optimization Methodology

The optimization methodology is based on two approaches:

1. Process optimizations are MINLP problems that are time-consuming efforts, initially to build robust models. In addition, they often lead to nonconvex optimization problems that do not converge to a global optimum. Moreover, as process systems of chemical plants have a strong nonlinear behavior, bifurcations and also multiple steady states often occur. Another limitation to MINLP problems is that the superstructure selection is not a trivial effort where alternatives are easily overseen. Despite these disadvantages, the quality of the MINLP problem solver and the superstructure selection will become more mature.
2. The evaluation of optimized alternatives: this is applicable when the number of alternatives is limited.

Both methods are applicable, and are sometimes combined where the MINLP solving is initially used to reduce the number of alternatives. With a reduced set of alternatives, NLP optimization is applied and the alternatives reduced by evaluation.

A *layered* approach is selected for optimization, that fits in the process synthesis methodology (Figure 4.3). The optimization layers are projected over the process synthesis methodology as is shown in Figure 4.4. Such a layered approach has the

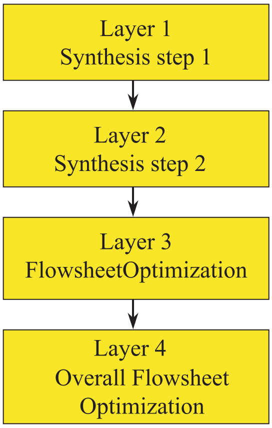


Fig. 4.3. A layered optimization approach.

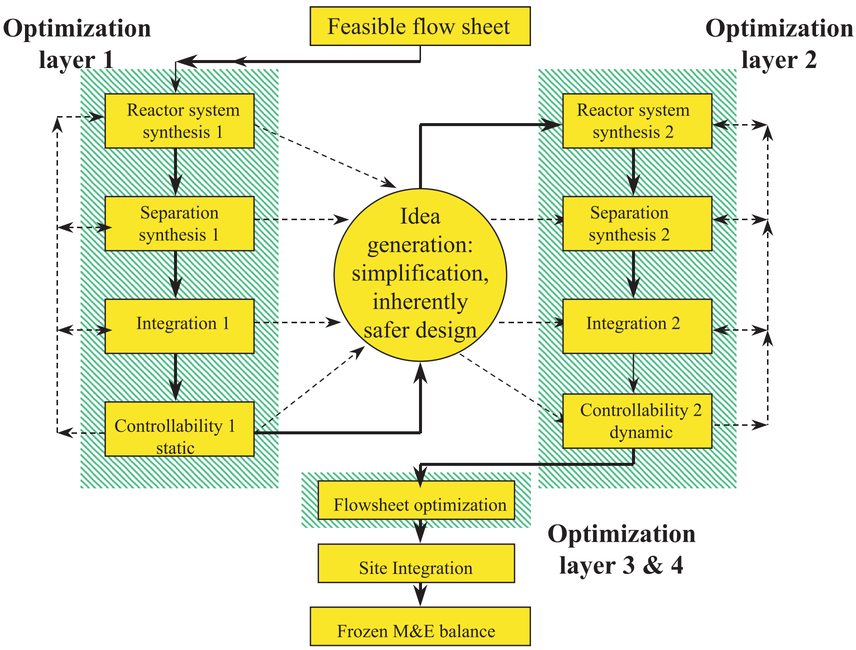


Fig. 4.4. Process synthesis: methodology including layered optimization.

advantage that design engineers can follow the evolution of the optimal design and understand the impact of design decisions. The design engineer must model all the process alternatives in the simulation/optimization. By using this layered approach he/she receives the intermediate results for evaluation. The optimization approach as discussed has four successive layers, each of which will gradually increase the size and details of the models and adapt the optimization (objective) function. The number of alternative options is reduced as the decision tree is descended (Figure 4.5), while the number of DOFs seen as relevant to the problem is reselected.

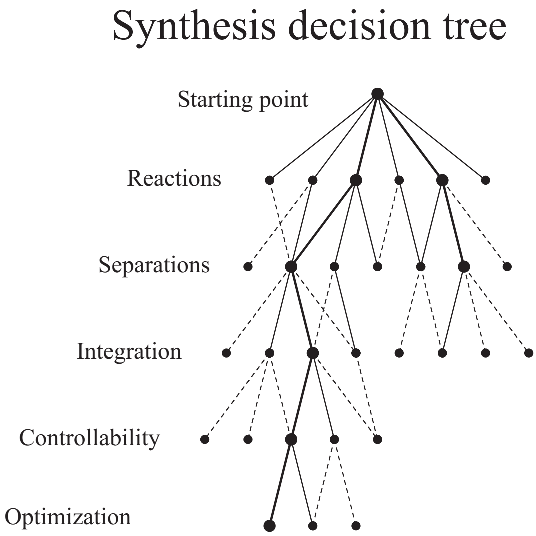


Fig. 4.5. Synthesis decision tree for a process plant.

The synthesis is initially performed as per process sections (see Section 4.1.4). To cope with the interaction between these sections it is necessary to optimize the intermediate stream compositions and price setting, this can be done by a few manual iterations in a synthesis step(mostly carried out during optimization layer 2 and 3). Iterative calculations might be minimized by assigning a cost and capital value to a recycle stream as was mentioned under the economic section. Ultimately, the complete process must be optimized after combination of the sections, and this will be done with a limited set of DOFs per section.

4.1.5.1 **The first layer**

The first layer relative to the reaction includes separation and integration synthesis steps 1. The intermediate prices are determined (as discussed in Section 4.1.4). For the energy prices, the site energy prices are taken initially at thermal energy levels relevant to the application.

Simple and surveyable methods are preferred to discriminate between alternatives which is the main effort in synthesis step 1. For reactors, discrimination can be made between CSTR(s)/PFR(s) or a combination of these, including a preliminary energy configuration based on variable margin. This is comparable with the attainable region approach as discussed by Biegler et al. (1997). The difference is that in the proposed approach the alternative solutions are compared on a variable operating margin.

Separation selection can be carried out through heuristic rules, or on cost comparison, while for sequencing of distillation columns, minimization of the marginal vapor flow provide good results (Biegler et al., 1997).

It was noted previously that most practical process synthesis studies have limited alternatives due to constraints and gradual technology developments. In many cases, each alternative might be evaluated individually and compared with other alternatives to avoid solving a MINLP problem. For a larger set of alternatives, MINLP is the way to proceed.

Integration studies in this layer emphasize the integration of:

- process streams, by taking advantage of less purified streams (including streams as hydrogen which might form part of an overall network); and
- utility streams as energy, process water, cooling, refrigeration.

The constraints for integration need to be defined, although at this stage they are preliminary. Integration studies are used to calculate the target consumption for the flowsheet under study, while options are exercised to achieve lower targets by manipulation of the process conditions. The outcome of the optimization layer 1 is a limited set of process alternatives for further evaluation.

4.1.5.2 **The second layer**

The second layer during synthesis step 2 is also divided into reaction separation and integration. The intermediate prices are updated, while the energy prices are kept at the site energy values.

In this layer each alternative is optimized at the maximum achievable NPV. This means that the cost estimation section and the optimization section for DFC and NPV calculation has been connected to the simulator. The cost estimation functions need to be adopted in the working areas to create continuous behavior, and also to avoid discontinuities. (Most cost estimation databanks have discrete cost data against equipment size.)

Mixed integer problems are to be avoided, so a continuous optimization problem is created, and a stage-to-stage calculation method as quite common used for rectification which apply integers (number of stages) isn't prefered. Modeling is preferably carried out with short-cut models as applied for distillation by Fenske–Underwood equations. For extraction, Kremser equations are used to describe the unit operation. Separations such as distillation, extraction, stripping, and absorption can also be described in mass transfer functions to avoid the equilibrium model description.

For the reactor system the selected CSTR/PFR combination is branched into alternative designs where the process simplification has its major input, see Section

4.2.1. To minimize the optimization effort the number of DOFs for the alternatives are minimized to those which have a major impact. The operating area is also bracketed, though care must be taken that it is not narrowed too much.

For the separation section the inputs are the selected separations and the preliminary sequence of separations. Now, constraints are defined based on the safety, environmental data and the static controllability studies. A preliminary sequence and constraints evaluation eliminates those alternatives that are far from obvious. The next step is to generate a complete list of remaining alternatives, including integration alternatives based on the target study, for further evaluation on NPV. The process simplification options need to be introduced at this stage. The number of design and operational DOFs is limited by arbitrarily selecting pressure and separation specification for those streams which are determined economically. Comparison of the optimized alternatives brings us into the position of selecting the best competing flowsheets. At this point, preliminary equipment sizes are known as well as the DFC and NPV.

Integration in this layer is repeated, but limited to the selected best flowsheets. The constraints need to be revisited and further defined, such as utility conditions and back-up provisions in network situations. The target studies will be extended with the targets for heat exchange areas and number of units. The selected flowsheets will be subject to sensitivity (flat or steep optimum) and variability studies regarding price sets of product and energy. The final selection for the flowsheet is then carried out.

4.1.5.3 The third layer

The third layer of calculations during the flowsheet optimization synthesis step is performed section by section, with updated intermediate stream compositions and prices. The prices for thermal energy might be different depending on the temperature/pressure level. These prices can be determined in relation to the primary energy price by calculating the net effect on primary energy consumption by incremental or decremental heat consumption at the specific level. At this point of the design, it is important to know the process integration in relation to the site energy system.

Modeling is preferable carried out rigorously, but mixed integer problems should be avoided (see Section 4.1.5.2). It should be noted that, for example, the feed point selection for the distillation is not optimized during this layer, but this will be done during the detailed process design. Now, all relevant operational and design DOFs are set free, including pressure and separation specifications, while all constraints must be reinspected. Some DOFs may be fixed in order to simplify the problem. In the case of a distillation tower, at optimization layer 2 the reflux to minimum reflux ratio is set free in layer 3 these might be fixed. At layer 3, when the energy prices are the same and the specification is close to its layer 2 assumptions, these might be fixed. The same applies for a reactor system, when for example the reactor pressure and catalyst volume had no significant effect on the NPV, it might be decided to fix these at layer 3. The selection of the relevant DOFs can best be supported by a sensitivity analysis and its effect on the NPV. In case of any doubt, the DOFs should be set free. All optimizations are carried out on economic performance as NPV. As prices will vary over the lifetime of the project, sensitivity studies will be executed after the majority of the design is fixed in order to evaluate the impact of these circumstances on operation and any significant design parameter.

4.1.5.4 The fourth layer

In the fourth layer, which is the successive activity during the optimization synthesis step, optimization is performed for the whole process. The intermediate prices and energy prices are updated. The reaction and finishing sections are combined, and the overall process is optimized at this point. The DOFs are limited to all operational DOFs and some major process design parameters such as reactor dimensions and major recycle equipment dimensions. Most design parameters will be fixed, for example the number of theoretical stages for separation columns and the overall heat/mass transfer coefficients will normally be fixed. The intermediate conditions between the subsections need to be verified with those used during layer 3. A large deviation might mean that layer 3 has to be repeated. The process sections are combined for the ultimate process optimization. In this case, the combined sections are optimized as one overall process with the operational DOFs and the major design parameters free. It will be clear that robustness of the model is a primary requirement, particularly if more recycle loops have to be closed. The optimization is concluded by varying the prices to judge the impact on operational as well as major design parameters. The model might be used as a basis for an operational optimization model.

Summary

- The methodology for optimization is built up on a layered approach. This gives the engineer valuable feedback on the model building and process design evolution. As MINLP optimizations are not yet robust in commercial software, the concept also follows the evaluation of individual optimized alternatives, although both methods are applicable.
- The methodology is based on four optimization layers. Each higher layer will gradually increase the size of the models (more detailed), and increase the optimization accuracy, but reduce the number of alternative options while descending the decision tree and select the number of DOFs as relevant for the problem.
- The first layer to be executed during synthesis step 1 is supportive to:
- selection of the reactor PFR versus CSTRs or combination;
- selection of the separation techniques; and
- pre-selection of the separation sequence.

The optimizations are based on the evaluation of alternatives within a process section with comparisons of operational costs for reactor type selection and distillation sequence selection. Only in specific cases might capital cost be introduced.

- The second layer to be executed during synthesis step 2 is supportive to:
  - selection of the reactor configuration;
  - ultimate selection of separation sequence; and
  - determination of the preliminary operational conditions and equipment dimensioning.

The continuous optimizations are based on DFC/NPV calculations with a limited set of DOFs for the preliminary design of process sections. Modeling is carried out based on short-cut (reduced) models to achieve rapid solutions, but also to avoid mixed integer problems as introduced by equilibrium stage-to-stage calculations.

- The third layer is after the final flowsheet has been selected, to determine the overall equipment dimensions and operational conditions for the process sections

The continuous optimizations are based on DFC and NPV calculations with a maximum set of design and operational DOFs for the final flowsheet.

- The fourth layer of optimization is performed on the overall process. Its primary purpose is to verify the results of the process section in the overall process. The impact of price variations on the design and operation are evaluated at this stage.

The optimizations are based on DFC and NPV calculations with a reduced set of DOFs per section, covering major equipment dimensions and all operational DOFs.

4.1.6
Creativity

The most important aspect of process synthesis is creativity, because that is the way to achieve competitive designs. It is during the simplification / idea generation where creativity plays a dominating role. Creativity begins with recognizing an opportunity – when people recognized the need to wipe the car's windscreen, someone invented a screen-wiping mechanism. A similar comment might be made about the building of an airplane having been derived from an interest to fly. Most new things or inventions come from a recognized opportunity, or:

Opportunities are the nutrients for creativity.

The opportunity to design simple and robust plants that are competitive, is a challenge, and in order to achieve this much alternative thinking is required. That does not necessarily mean that new things *will* be invented – often it is simply the right combination of known elements that clicks into place and leads to a new invention.

Creating new things is more often based the combination of known elements than by inventing something new

The design of simple process plants can be realized in many alternative ways – the challenge is to select the right combination of known operations to design an optimal process. The invention of new things occurs at the research phase of a project – at the design stage, we have to apply what we know. The creation of alternative solutions to a design problem, and the selection of the best solution, is the way to go – or in other words:

Think in alternatives and select the best

The development of alternatives is often best carried out in structural brainstorming sessions, as a team effort. Although this an effective way to collect ideas, it is often a one-time effort. At the same time, the approach is self-limited by the target set by the leader. One handicap with engineers is that they are trained to solve problems in a sequential manner. This was helpful when trying to understand the rather abstract world of process engineering. Building a process flowsheet always comprises a sequence of activities such as pump, heat, separate, cool, pump, etc. It is this sequential thinking that must be broken in order to achieve simple and robust facilities.

Sequential thinking is way to order and understand things but it can be a handicap for the search of integrated solutions.

There is more to brainstorming than simply sitting together in an open-minded setting and letting the creativity flow. Creativity needs time, for people to open their minds, and for unrestricted stimulation. Experience teaches us that it is very easy to collect standard or common ideas for improvements, but very difficult to collect good ones. Time and a stimulating environment are essential.

The death to creativity is putting people under time pressure

Another factor that is counterproductive to creativity is *irritation*. People involved in a project will not – and cannot – contribute to creativity when they are irritated, as such a mental condition is simply not the right climate in which to be creative. The working environment provides a major contribution to creativity. It was Thomas Alva Edison who created a motivated team to explore new techniques related to the applications of electricity and electro-mechanical devices. Indeed, it was Edison who explained geniality:

What people call geniality is simple hard work: one percent inspiration and ninety nine percent perspiration.

The acceptance of an idea is too often more cumbersome than its development. This is one of the advantages of developing a creative climate in a team, and that was one of the strong points of Edison's team concept. The acceptation of ideas within a team is higher, as it is perceived to be a joint effort. It was Herbert Dow (the founder of Dow Chemical) who phrased the cumbersome way to achieve implementation of new ideas as follows:

I can find a hundred men to tell me an idea won't work, what I want are men who will make it work.

Creativity is an activity which can be stimulated in brain storming exercises by means of a technique called functional analysis as discussed in **Chapter 10.** Reference need to be made to process knowledge but also to simplification techniques as discussed in the following chapter.

Summary

The lessons to be learned for synthesis teams with regard to creativity are:

- Be aware of the opportunities for designing competitive plants based on the simple and robust concepts.
- Motivate the development team in being creative, and challenge the team at the synthesis steps of the project to come up with creative solutions – but leave time for implementation.
- Sequential thinking in solving problems is a barrier against finding integrated, operational solutions.
- Set up brainstorming teams during different phases of the synthesis work to generate the maximum number of ideas, and have them evaluated by the team itself.
- Be aware that selling new ideas is much more difficult that creating them.
- Creativity resulting in design improvement alternatives can at best be excersized in brain storming sessions..

4.2
The Methodology of Process Synthesis

The starting point for a conceptual design (including a process synthesis study) is a technical feasibility study for a project, as mentioned previously. The feasibility study, which is based on process simulations and economic cost, compares the different technologies and selects the best technology for the project. The selected technology also emphases a feasible flowsheet

The first elements to be collected and completed during the synthesis work are:

- The physical and chemical properties.
- The constraints (see Section 4.1.2).
- The reactor and separation models for the selected technology, based on the feasible flowsheet.
- The unit ratios and the DFCs and NPVs of the different sections of the selected technology, based on the feasible flowsheet

In the following paragraphs, the methodology is followed as shown diagrammatically in Figure 4.1 and Table 4.1.

4.2.1 Reaction

4.2.1.1 Evaluate raw materials, reactants and products and the chemical reaction

The first decision to be taken is that of which feed streams are to be selected for the main reaction, in addition to other purposes such as solvent, anti-oxidant, inhibitor, neutralizing agent, and the physical state of the materials. All of these chemicals must to be evaluated on:

- Purpose
- Safety – internal as well as external
- Environmental
- Transportation mode, storage, and its physical state
- Integration in relation to other processes
- Purity and concentration

These steps are often under estimated, although a large proportion of the costs are logistic cost which are determined – but not yet quantified – at this stage. Some of these materials are not selected at this point, though it is possible to discuss them here as they all have to pass the same rationale.

- The *purpose* often leaves us alternatives: for example, if we want to neutralize with a base, there are often more alternatives such as caustic solution or pellets, lime, NH_3, a weak inorganic or an organic base. Similar choices are to be made for acid neutralization. In most applications alternatives are available, including the main reactants. List all these alternatives from economic, safety and environmental perspectives – and do not forget to list the form/concentration of supply.
- Apply the inherently *safer* and *environmentally sound* design philosophies at this stage to their full extent. It is at this point when there is the major impact on the safety and environmental aspects of an operation. A striking example of this is the selection of a chemical: in an operational facility, seawater was used for direct cooling of process streams, but the seawater needed to be treated to overcome the growth of mussels within the exchangers. Although the solution was to add chlorine, it was unnecessary to highlight the inherent danger of having chlorine on site; rather, a solution of sodium hypochlorite was found to be a suitable replacement.
- *Transportation* and *storage* each have major impacts on the design. The example of the batch plant in Figures 1. 4–1.7 in **Chapter 1** clearly shows the increase and decrease of storage facilities during the process' evolution. The practice of transporting a dosing agent in dedicated containers in a liquid form at a concentration level for easy handling is to be preferred. It should be recognized that handling operations can lead to mishaps and are to be minimized.

- *Purity* is another main point for discussion. The raw materials may come from different suppliers, or from "own" sources as existing processes at location. The overall input and output balance of the process as proposed by Douglas (1988) is a key factor at this stage. It is vital to understand the effect of an impurity on the reaction(s), as well as its potential for accumulation in the process. There may be significant advantages in using less pure streams as reactant or as product. An example is the use of lower-grade ethylene and propylene for alkylation reactions. Lower purity options are particularly important for components and its impurities that are difficult (high cost) to separate (see Section 4.2.3.2 Process integration).

It is not always practical to evaluate these materials at the beginning of the process synthesis step, but evaluation and selection should be ensured during the conceptual design.

4.2.1.2 Evaluate reactor type, excess of reactants, and options to shift the equilibrium, including simplification

Reactor system synthesis 1 inputs include:

- Chemistry
- Catalyst system
- Phase(s) of the reaction
- Reactor models

The generic factors influencing a reaction are:

- Temperature on kinetics and equilibrium.
- Pressure on equilibrium.
- Diluent on equilibrium, by lowering partial pressure and as heat carrier.
- Reactant ratio on kinetics, equilibrium, as heat carrier.
- Catalyst concentration on kinetics.
- Time on conversion.

The objective is to compare different reactor configuration as CSTR(s) and PFR or combinations based on the variable operational margin to enable discrimination between different configurations. The variable operational margin is the difference between the revenues minus the costs of the raw material and the energy. In the case of a small difference occurring between alternatives, it is possible to proceed with two or three configurations for reactor systems.

The optimization requirements should be determined as:

- Economic prices of inlet and outlet (process and utility) streams (see Section 4.1.4).
- Constraints
- Preliminary energy exchange system in reactor section.
- Process conditions to be fixed. Depending on the effect on the reactor configuration selection, those conditions are fixed that have a low impact, for example reactor pressure for liquid or pressure-neutral reactions, or systems

where a practical pressure limit becomes effective, such as for vacuum systems, temperature for reactions with low energy effects and low activation energy. The intention is to limit the size of the optimization problem
- The DOFs might be the ratio of reactants, ratio of diluent to reactants, conversion, inlet temperature, pressure and reactor configuration.
- The outputs are the selected reactor type of CSTR/PFR or combination, with the restricted optimized conditions by the selected DOFs.

4.2.1.3 Reactor simplification

The starting point for this activity is the research data for a certain reactor and catalyst type described in a model. The objective is evaluation of the most promising reaction configuration. The evaluation will initially be performed based on the assumed conversions as applied in the feasibility flowsheet. The generation of alternatives with an emphasis on simplicity is now crucial. The following points for simplification will be discussed and illustrated with some examples:

- Simpler reactor configurations
- Larger-scale reactor systems
- Combination of reaction and separation

Simpler reactor configurations This may be illustrated with some typical industrial examples of simplified rector systems from a configuration perspective:

1. Replacement of a loop reactor with six exchangers by a boiling reactor (Figure 4.6); this resulted in a high capital saving, while the selectivity and conversion were unchanged.
2. Replacement of three isothermal CSTRs in series by an adiabatic CSTR and an adiabatic plug flow (Figure 4.7). This concept also led to high capital savings with removal of the recycle heat exchangers and six circulation pumps, and the replacement of three vessel by one large vessel. The system was realized by a slight increase in one of the reactants. The lower conversion achieved was already over-compensated by energy recovery and a higher selectivity.
3. The modification of a series of CSTRs for nitration reactors by an adiabatic mixing street (Figure 4.8) (Hauptmann et al., 1995).
4. Other examples include the installation of multi-stage fluidized beds or a riser bed to replace fixed or fluidized beds, or the replacement of a series of CSTRs for gas–liquid reactions with multi-stage bubble reactors (Schluter et al., 1992).
5. The installation of reverse-flow reactors (also called bi-directional reactors) equipped with packing as heat exchanger, for adiabatic auto-thermal operation (Matros and Noskov, 1988; van de Beld and Westerterp, 1996; Kuczynski et al., 1987) compared with a packed bed with cross-exchangers (Figure 4.9).

Several multifunctional reactors are descibed by Westerterp 1992.

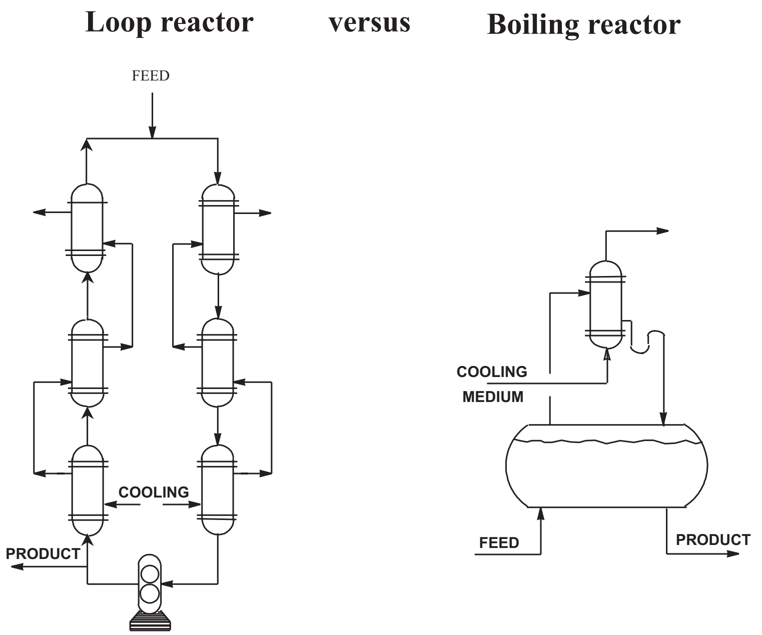


Fig. 4.6. A boiling reactor as replacement for a loop reactor.

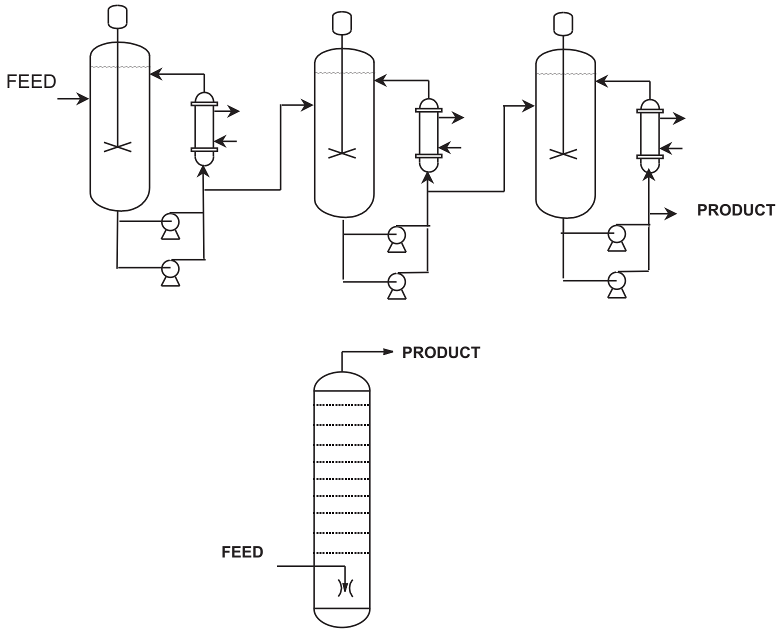


Fig. 4.7. Three isothermal CSTRs in series versus an adiabatic CSTR and an adiabatic plug flow in one containment for a homogeneous liquid reaction.

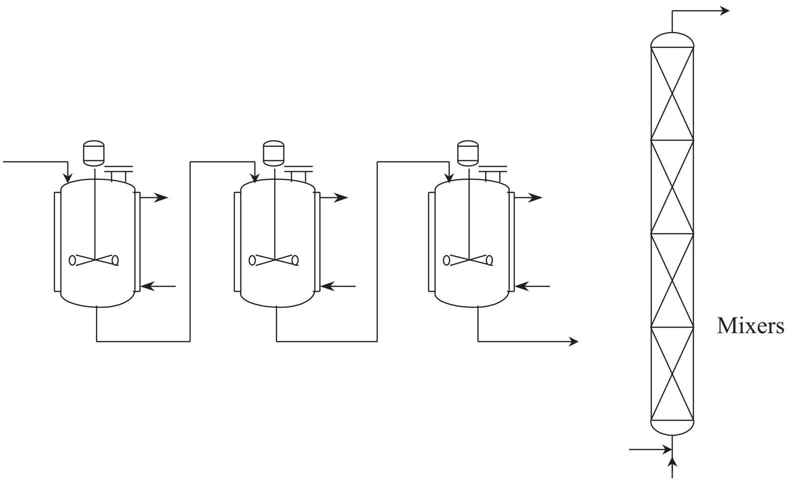


Fig. 4.8. Nitration of aromatics in CSTRs in series versus adiabatic mixers in series.

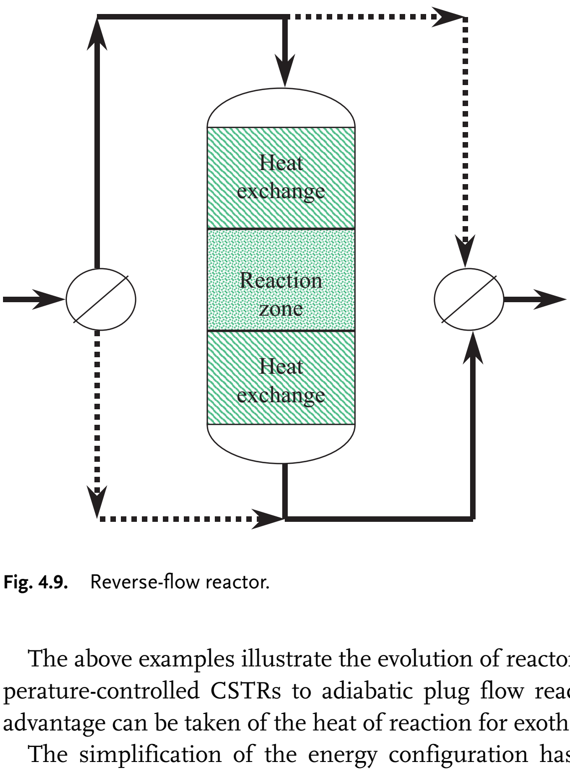


Fig. 4.9. Reverse-flow reactor.

The above examples illustrate the evolution of reactor design from a series of temperature-controlled CSTRs to adiabatic plug flow reactors. In this case additional advantage can be taken of the heat of reaction for exothermic reactions.

The simplification of the energy configuration has a major impact on reactor development, for example with reverse-flow reactors.

Larger-scale reactor systems Simplification can also be considered from a size perspective. Many processes are considered to be restricted by size, and therefore many reactor systems are doubled, tripled, or even quadrupled. A closer inspection of these systems shows that different types of constraint are in existence:

- mechanical design;
- mechanical fabrication;
- flow distribution; and
- process-wise, or a combination of these.

Styrene reactors are an example of a mechanical design that is constrained. Historically, these reactors consisted of a two horizontal bed configuration with a tubular reactor partly in between, heated by flue gas (Figure 4.10). The mechanical stresses between the tube sheets and the shell were a constraint on the size, as thermal stresses caused cracks to occur at the connection because of a difference in expansion during transient operations. The evolution took different paths. Two intermediate solutions were the development of: (i) a supported thinner tube sheet that resulted in an increase in reactor diameter from 3 m to 5 m; and (ii) a salt-heated system that permitted a lower temperature on the shell side. The result was a reactor with a diameter of >5 m. The next capacity increment was realized by the introduction of a radial bed reactor (Figure 4.10). The concept included replacement of the shell and

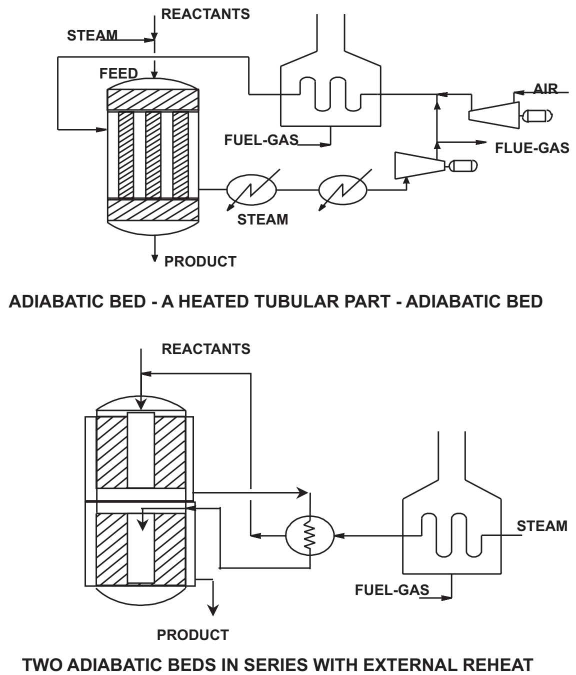


Fig. 4.10. The evolution of a styrene reactor system to achieve higher capacity.

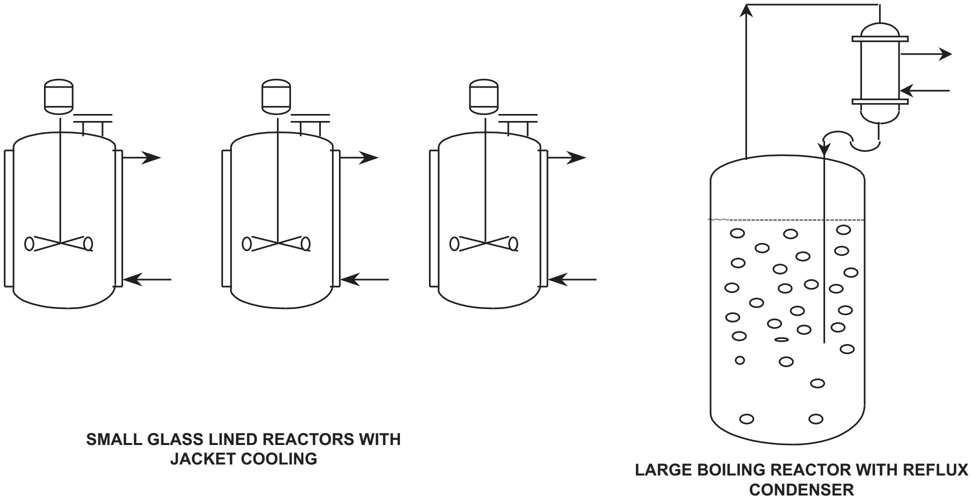


Fig. 4.11. Small reactors jacket cooled versus one large boiling reactor.

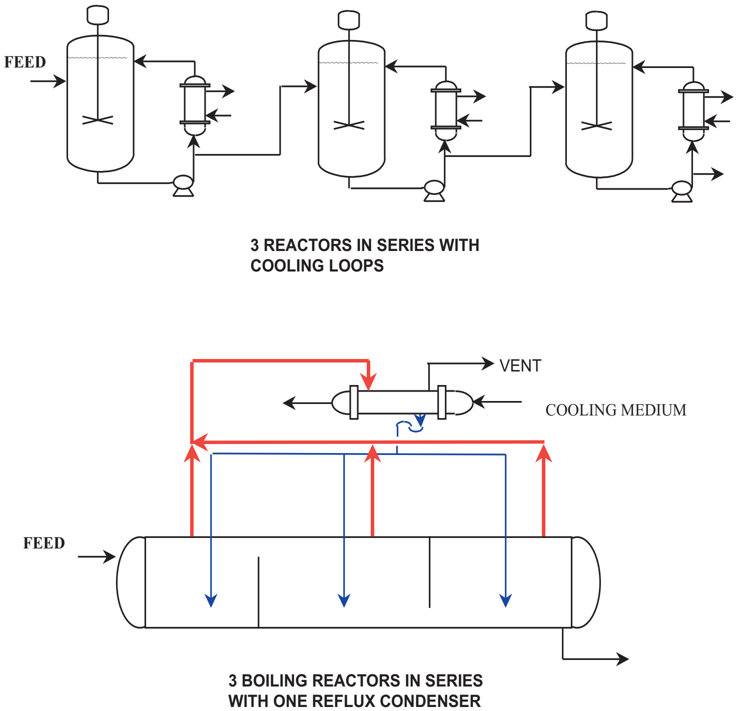


Fig. 4.12. Simplification of a series of loop cooled reactors by a compartmented boiling reactor vessel with integrated condenser.

tube exchanger in the reactor by an inter-stage heater. The problem to be solved was flow distribution at the inlet of the radial reactors, and the engineers were able to overcome this satisfactorily. By comparing both systems, it was clear that the energy system of the radial reactors with inter-stage reheat produced less lower-value energy (steam) and consumed power compared with the flue-gas heating system.

Another example of a mechanical constrained system is the glass-lined, jacket-cooled reactor. These are not limited by fabrication of the vessels, but by heat removal. The jacket surface area increases with the square of the diameter, and the content with the cube of the diameter. The solution was found (process wise) to involve the application of a reflux condenser (Figure 4.11).

Another variant of the boiling reactor is shown in Figure 4.12. In this example of simplification, three loop-cooled, agitated reactors are replaced by a boiling reactor vessel. The vessel is partitioned in three compartments and provided with one reflux condenser.

The capacity of steam-cracking furnaces is another example which over the years has increased by factors of 4–5 as a result of improvements in mechanical design.

Combination of reaction with separation This is another step in the consideration of simpler designs. During the past few decades, the process of reactive distillation – sometimes a catalytic distillation – has matured to a point where it is now considered where distillation of reaction products occurs in the same temperature range as the reaction. Factors that play a role in reactive distillation include:

- The reaction occurs in the liquid phase; it is often catalytically homogeneous or heterogeneous, S/L.
- Exothermic reactions have an advantage, as the reaction heat can be used for the separation. Endothermic reactions can also be applied, in which case the reaction heat must be added via a reboiler
- Equilibrium reactions have the advantage that conversion can be driven to higher levels by removing the products.
- Higher selectivity might be achieved by product removal to minimize consecutive reactions.

Several industrial applications of reactive distillation have been installed, for example etherifications like MTBE (methyl-*tert*-butyl ether) production, alkylations like the cumene process and esterifications like the methyl acetate production.

Other combinations of reaction and separation include: (i) the application of a zeolite membrane reactor (van de Graaf et al., 1999); (ii) countercurrent gas solid–solid trickle flow reactor for equilibrium reactions such as methanol synthesis (Westerterp et al., 1987); (iii) inter-stage product removal with absorbers in a methanol plant (Westerterp et al., 1989); and (iv) oxidative removal of hydrogen between the reactor stages of a styrene reactor. For more details on simplification, see **Chapter 5**.

Reactor system synthesis 2 inputs include:

- Results of reactor system synthesis 1,which is a pre-selection of reactor configurations.

- Separation selection 1
- Process integration 1

The objective is selection of the final reactor configuration and preliminary reactor size for the process; this is based on cost, DFC, and NPV results. In order for selection of the final configuration to be made, a careful evaluation of simplification alternatives must take place, incorporating:

- Updated economic prices for inlet and outlet stream after separation 1.
- Constraints.
- Updated energy exchange system after process integration 1.
- Cost estimation updated for local situation and provided with continuous function in the working area to avoid discontinuities resulting in converging problems.
- Fix reactor conditions which have a limited impact on the reactor system to reduce the sizeof the optimization problem.
- The DOFs to be selected might be reactor volume(s) temperatures, reactants ratios, diluent ratio, and catalyst concentration, or amount.

The results are the selected reactor system, including preliminary dimensions under restricted optimized conditions, restricted by the DOFs selected for optimization.

Summary

The selection and design of reactor configuration is the most essential step of the process synthesis, as this section largely determines the economics of the process with respect to the selectivity, conversion, and capital cost. The factors that play a major role in the design of the reactor section are:

- The safety aspects are largely dominated by the selection and inventory of the chemicals involved.
- The simplicity of the design will have a major impact on the capital and ease of operation.
- Simpler reactor designs evolve into the direction of adiabatic plug flow designs with maximum benefit of reaction heat, (see **Chapter 5**).
- Large single reactor train systems are evolving which benefit from the economics of scale, while the design is supported by detailed reactor, flow and mechanical modeling.
- The combination of reaction and separation is driving down the cost of process design, and leading to higher conversion systems.
- Synthesis stage 1 activities lead to the pre-selection of reactor configuration based on operational cost.
- Synthesis stage 2 selects the final reactor configuration and preliminary size based on the advantages of simpler designs and optimization of the system on NPV.

4.2.2 Separation

The development of a separation train for a continuous process is divided into three steps:

1. Selection of separation techniques.
2. Sequencing of separation techniques.
3. Adapting process conditions for integration and optimization.

The objective is to develop an elementary overall flowsheet that carefully shows which components need to be removed, and where they are expected to leave the process. The development steps will be discussed in order, although initially the overall task of separation section needs to be defined by what is known as the Douglas input and output structure of the flowsheet.

4.2.2.1 Develop an input and output process stream diagram

The input required for the stream diagram is a detailed component analysis of all feed streams (including all additives) and of the reactor(s) inlet and outlet streams. The stream diagram must contain external streams with quantitative and if not yet available qualitative component information, and also show the major recycle streams. As example, a flowsheet for an ethyl benzene process is shown in Figure 4.13. Even so when the component information is only available qualitatively, it is important information for the designer. All components that are either fed or produced must leave the process. The product specification and environmental requirements set constraints on the impurities leaving with the product stream and the purge streams. Emphasis must be placed on this point, as during development of the separation train the separation specification is often determined by impurity levels and less often by the major reactor components. The potential environmental

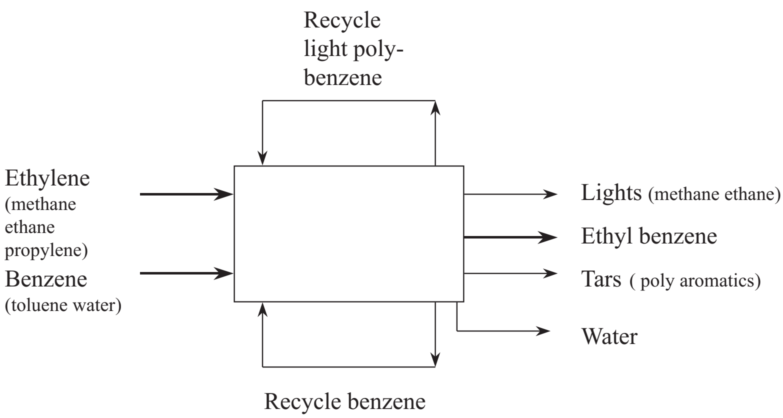


Fig. 4.13. Input and output diagram for an ethyl benzene process.

load streams are also identifiable at this stage. With regard to the ethyl benzene process, we need to know where impurities in the ethylene (e.g., methane, ethane, and propylene) leave the process. The impurities in the benzene (e.g., water and toluene) leave the process in the product and in a separate water outlet. An alternative might be pretreatment at the supplier versus in the process plant. It is not always known beforehand in which stream these impurities will leave the process, but the overall balance should focus on their removal.

4.2.2.2 Selection of separations

The selection of separation techniques (Douglas, 1988; Smith, 1995; Biegler et al., 1997; Seader and Henley, 1998; Seider et al., 1999) must be deduced from the physical properties, but also take into consideration the safety aspects. Thus, a list must be prepared of available physical and safety properties for the components involved, and their potential separations. If reliable information is missing, then estimation techniques may be used for the initial selection, but this needs to be confirmed later experimentally. Separations can be defined as either *heterogeneous* or *homogeneous*.

Heterogeneous separations These are governed by three basic rules:

1. Separation of different phases of a heterogeneous mixture is easier (lower cost) than for a homogeneous mixture.
2. Separation of the phases of a heterogeneous mixture should be carried out before homogeneous separation.
3. Larger particles/droplets are a preferable choice.

The constraints on phase separation provide a reasonable driving force (particle/droplet size and density difference) for separation, the phase separations for consideration being:

- Vapor–liquid
- Liquid–liquid
- Solid–vapor
- Solid–liquid
- Solid–solid

A number of different techniques are available for these varying phase separations. The selection of technique is often highly self-directing for different concentrations and particle/droplet sizes and distribution. In cases where the particle size formation is both understood and controllable – for example known crystallization kinetics, grinding, and/or cutting – the direction is to choose particles of larger size.

Homogeneous separations Homogeneous separations can only be performed by the addition or creation of another phase; examples include distillation, extraction, and adsorption. Homogeneous separations can be further subdivided into gas and liquid separations.

Gas separations These are mostly limited to:

- pressure distillations (including partial condensation);
- cryogenic distillations;
- absorption;
- adsorption/chemisorption;
- membrane; and
- reaction.

Pre-selection guidelines are:

- To remove selectively one component with absorption/desorption. Examples are: (i) the absorption of ethylene oxide from the reaction gas into water, or of methanol from syn-gas; (ii) chemical absorption/desorption for application without available selective solvents, such as CO_2 and H_2S removal from refinery and synthesis gases; (iii) NO_x and SO_3 conversion in nitric acid and sulfuric acid processes, respectively.
- Concentrate selectively a component through adsorption/membrane, e.g., hydrogen from methane. This is a standard application for a pressure swing adsorption (PSA) unit.
- Separate components with dew points of gases around ambient conditions not lower than –40 °C through pressure distillation, e.g., distillation separations of C3 and C4 streams.
- Separate components with low boiling points ≤40 °C, e.g., cryogenic distillation, such as C1 and C2 separations, air separation. Hydrogen is an exception due to its very low boiling point.
- Remove low concentrations of components with absorption/adsorption/chemisorption, e.g., hydrocarbons (odor, toxic, environmental components) removal from vent gases.
- Remove components without the availability of a selective medium through reaction, e.g., hydrogenation of acetylenes or di-olefins from olefins, the removal of NO_x from flue gasses, catalytic incineration of hydrocarbons.

The above guidelines are to be used as pre-selection for gas separations, though ultimately the final selection must be carried out after the evaluation of alternatives on the basis of NPV.

Liquid separations The most commonly used liquid separations for homogeneous systems are:

- distillation, including evaporation/condensation;
- extractive and azeotropic distillation;
- extraction;
- adsorption/chemisorption;
- crystallization;
- membrane; and
- reaction.

The standard separation technique for homogeneous liquid systems is by simple distillation (separation on two key components). There are several reasons why distillation/evaporative separations are a first choice:

- Distillation is a well-known and proven technique which can easily be designed based on vapor liquid equilibrium data. These data are widely available from data banks, and prediction techniques of these data also gained confidence for preliminary designs at synthesis stage 1.
- Distillation separations can be performed very sharp on the key components, and generally does not require an additional unit for purification.
- Distillation is carried out in one unit; other separation techniques need more units to achieve separation.

The disadvantages of distillation are its limitations for the separation of temperature-sensitive materials, and its high capital and operational costs.

Extractive distillation is often applied when the relative volatilities are low (<1.1) and conventional distillation would result in over 100 theoretical trays with very high reflux ratios over 10. The disadvantage is the much higher investment cost, as an additional tower is required for separation to be effected.

When *extraction* is compared with distillation, an extraction unit always requires purification of the extract, and of the raffinate from the solvent. Similar arguments are valid for extractive distillation, and adsorption. For extraction, an additional point to overcome is that tests are required to size the height of a theoretical separation stage and to judge its tendency to emulsify due to the presence of minor impurities.

When comparing *crystallization* with distillation, the design of a crystallizer requires crystallization kinetics to be applied that are seldom available to good-sized crystals, and the crystals formed often need to be freed from the mother liquor. When the final product is needed in crystalline form (e.g., sugar), there is no alternative technique available.

Membrane separations have a limited application area due to several reasons: the competitiveness of the membrane with the feed streams; fouling characteristics; temperature sensitivity; and cost of the modules. Despite this, membranes are being increasingly applied in the field of water purification.

Reaction is often used as a last resort if all other techniques fail to perform, or are highly priced. An exception must be made for ion exchange, which is in widespread use but is already facing competition from membrane separations in water purification systems. Low-purity product streams which can be sent to a downstream plant where separation takes place in the reactor by selective removal of the target product. This is an example of process integration.

Pre-selection guidelines are:

- For separation of main components with relative volatility >1.1, distillation/evaporative separation should be used.
- For separation of main components with relative volatility <1.1, extractive distillation/extraction/reaction should be considered. Examples include butadiene and benzene extractive distillations, and hydrogenation in olefin processes.

- For separation of low concentration (<1%) components, evaluate distillation versus selective absorption/stripping/adsorption/chemisorption. Examples include drying of hydrocarbon streams, removal of color or deactivating components, and removal of CO_2 and H_2S.
- Breaking of azeotropes requires evaluation of the following generic techniques:
  - Heterogeneous systems with water are preferably separated by simple distillation and decanting at the reflux drum of the minimum azeotrope (Figure 4.14). The technique involves only one column, but its application is restricted to situations where solubility of the top product is limited. An alternative (even more simple) method is to operate it as a stripper with open steam in the bottom, and to recycle the overhead stream back in the process; the overhead stream is then condensed and decanted into existing equipment. The disadvantage of open steam is that the water must leave the system at some point, which requires cleaning. Typical examples are the drying of hydrocarbons which form minimum azeotropes with water.
  - Homogeneous azeotropes can, as a first choice, be separated through distillation at different pressure levels. The pressure may alter the azeotropic composition, after which separation is carried out in a two-column configuration.
  - More extended separation techniques include: (i) azeotropic distillation with a separating agent (called an “entrainer”); or (ii) breaking the azeotrope by removal of one of the components with extraction. The latter method is often applicable in systems with polar and nonpolar components (a polar component such as methanol is easily removed using water as the extraction medium).

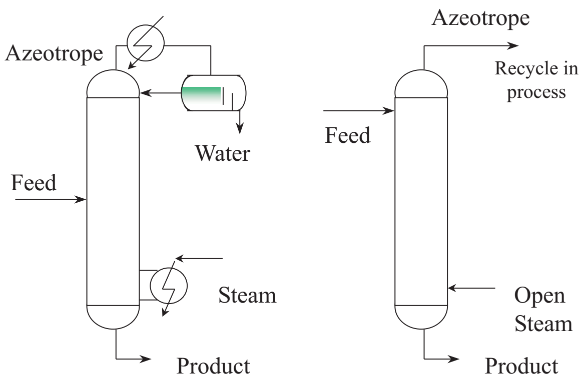


Fig. 4.14. Separation of a heterogeneous azeotrope in one column.

4.2.2.3 Sequencing of separations

The sequencing of separation is generally considered to be a MINLP problem, the argument being that the number of sequences to be evaluated grows progressively with the number of products and the number of alternative separation techniques.

If it is assumed that the separation technique has been selected, the number of sequences is still considerable. Table 4.2 shows this for a selected separation technique and an increasing number of products to be separated. In practice, the number of products to be separated after a reaction step are mostly between three and five, and in a chemical process this might be followed by successive reaction steps with their separation sections. The number of constraints for such a separation train is also considerable. In the example of Koolen et al. (1999) the number of sequences for five products was reduced from 14 to 9 due to constraints. In these situations – which cover most of the industrial cases – it is more practicable to optimize and evaluate all potential sequence alternatives rather than to define an overall optimization problem.

Table 4.2. The number of possible sequences for using a selected separation technique versus the number of products to be separated.

Number of products	*Number of separators*	*Number of sequences*
2	1	1
3	2	2
4	3	5
5	4	14
6	5	42
7	6	132
8	7	429
9	8	1430

In the previous paragraph, the separations were selected and the layout of the sequential steps can be presented in a generic superstructure (Figure 4.15) (Douglas and Stephanopoulos, 1995). This superstructure was compared with several flowsheets of well-developed processes, and the structure fitted reasonably well. The superstructure also respects the heuristic rule of "heterogeneous before homogeneous" separations.

Pre-selection of the sequence in the case of a distillation train – which always is a key activity during separation step 1 – is based on the selection of a minimum vapor flow alternative. This concept has been proposed by Porter and Momoh (1991), and reflects operational cost as well as capital cost. These authors have also demonstrated that the rank order of the total vapor flow is similar to the rank order of the total cost. This method is preferred to a heuristic approach. For each alternative, an overall mass balance is made where the separation specifications are either set by the final product requirements or are selected arbitrarily, whereupon these last specifications will become free at a higher level of optimization. The sequences under evalua-

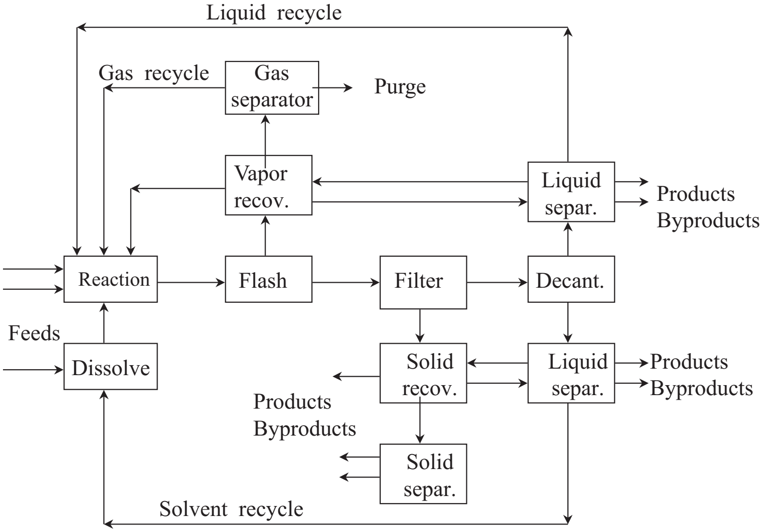


Fig. 4.15. General structure of a separation section (Douglas and Stephanopoulos, 1995).

tion are simulated at a reflux R to minimum reflux ratio (R_{min}) of 1.1 The vapor flow (V) is determined for each column by

$$V = D\,(1 + R/R_{min} \times R_{min}) \tag{1}$$

where R_{min} is calculated based on the Underwood equation for the key components:

$$R_{min} = \frac{1}{\alpha - 1}\left(\frac{X_{DLK}}{X_{FLK}} - \alpha \frac{X_{DHK}}{X_{FHK}}\right) \tag{2}$$

where α is the relative volatility between the key components;
X_{DLK} is the molecular fraction of light key in distillate;
X_{FLK} is the molecular fraction of light key in feed;
X_{DHK} is the molecular fraction of heavy key in distillate; and
X_{FHK} is the molecular fraction of heavy key in feed.

This formula can be simplified for a sharp separation, where the light key and lighter than light key leave at the top, while the heavy key and heavier than heavy key leave at the bottom. In that situation the equation is reduced to

$$R_{min} = \frac{1}{\alpha - 1}\left(\frac{X_{DLK}}{X_{FLK}}\right) = \frac{1}{\alpha - 1}\left(\frac{F}{D}\right) \tag{3}$$

where F is the feed and D the distillate flow rates.

Combining Eq. 1 with Eq. 2 gives

$$V = D\left(1 + \frac{R/R_{min}}{(\alpha - 1)}\frac{F}{D}\right)$$

Only light keys components and lighter go to the distillate F_{lights} and heavy keys and heavier F_{heavies} go to the bottom. F_{lights} and F_{heavies} are introduced as the sum of respectively all lights light and heavy feed components.

$$F_{\text{lights}} = F_A + F_B + F_C + F_D + \cdots\ F_{LK}$$

$$F_{\text{heavies}} = F_{HK} + \cdots\ F_X + F_Y + F_Z$$

$$F = F_{\text{lights}} + F_{\text{heavies}}$$

Now, Eq. 4 can be rewritten as

$$V = F_{\text{lights}} + F\,\frac{R/R_{\min}}{\alpha - 1}$$

Based on the vapor flow of each column, summation of the vapor flows of all columns gives the overall vapor flow. This must be calculated for each sequence to enable selection of the most promising sequence. The above approach is not limited to simple distillation – complex distillations can also be evaluated in the same manner.

4.2.2.4 Simplification of separation

The most obvious candidate is distillation, since this is one of the most utilized separation techniques and has high capital and operational costs. A practical example may be taken of a process with a reactor and distillation train. The boiling range of the components to be separated are shown in Figure 4.16. Note that there are two types of lights, each with different boiling points. In this particular example the feed to the reactor system contained lights which are inert for the reaction, but which are included in the separation scheme.

The distillation train for this mixture of seven components for separation is shown as a five-column separation flowsheet in Figure 4.17. A heterogeneous azeotropic distillation is included in the last column to remove water. Based on this scheme, different steps are shown in the idea generation, as presented in Figures 4.18–4.20.

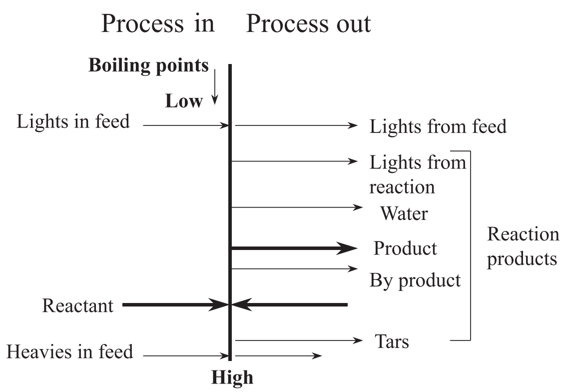


Fig. 4.16. Boiling points of inlet and outlet streams of distillation example.

- The first generation scheme converts the first separation after the reactor into a side draw column which removes unconverted reactant and tars in one column; the side draw had to be removed as a vapor to reduce the tar content. In this case the flowsheet is reduced to four columns.
- The second generation flowsheet combines the first column with the one after the reactor by installing a three-component distillation (a divided wall column; Kaibel, 1987).
- The last two columns are also replaced by a divided wall column; now, the flowsheet is reduced to three columns.

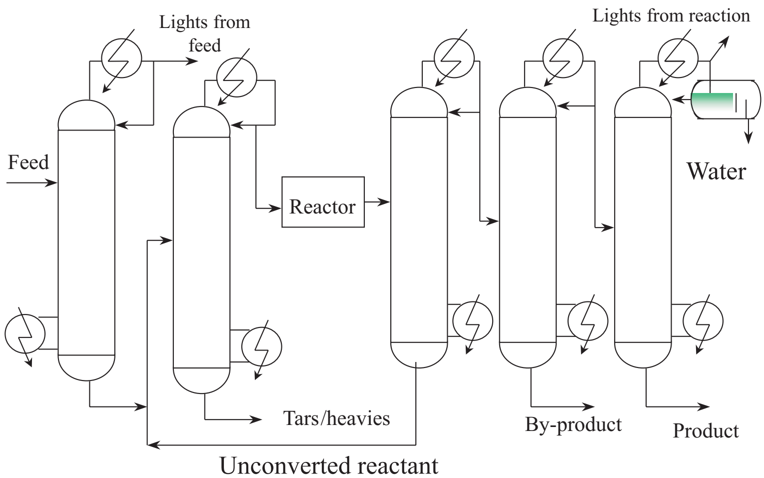


Fig. 4.17. Conventional distillation scheme: 1st generation.

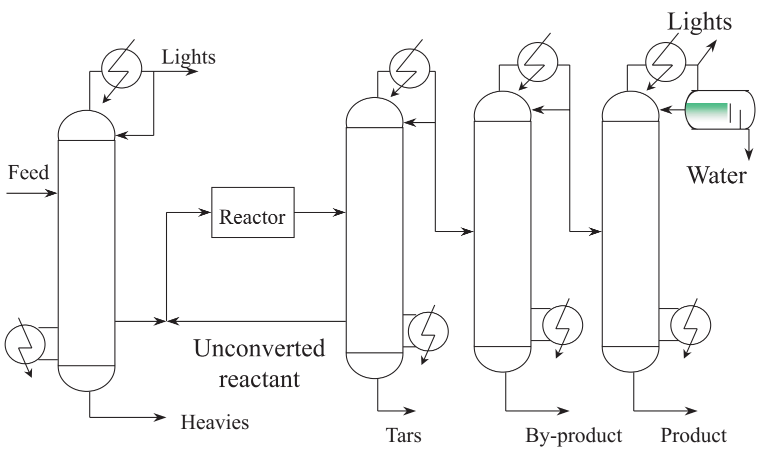


Fig. 4.18. Distillation scheme: 2nd generation.

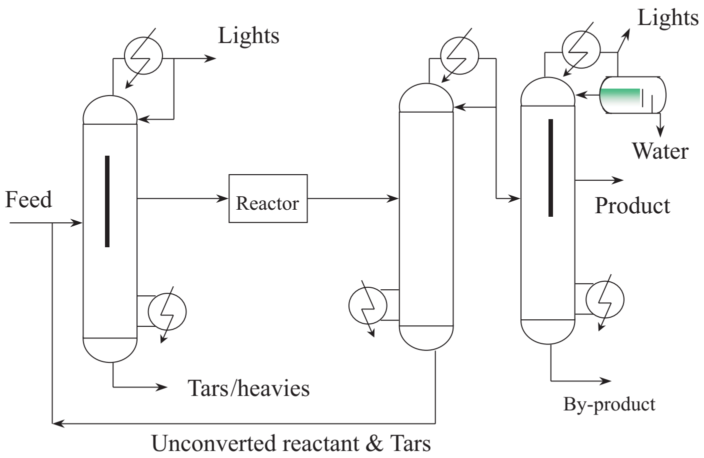


Fig. 4.19. Distillation scheme: 3rd generation.

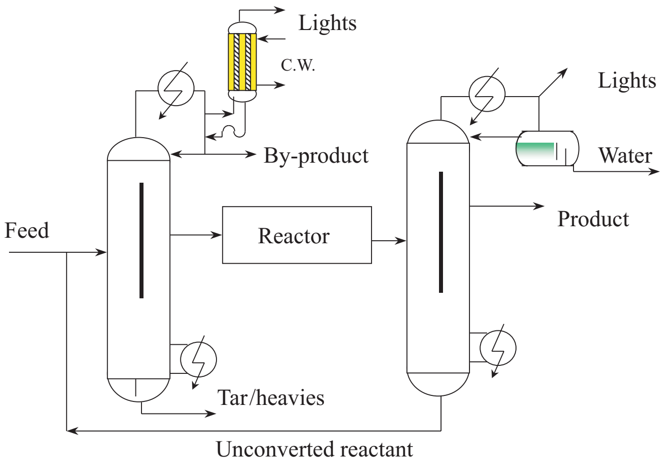


Fig. 4.20. Simplified distillation scheme: 4th generation.

- The third generation flowsheet converts the flowsheet into a two-column concept where the first column is equipped with a dephlegmator (a partial condenser with rectification). This flowsheet is a very reduced concept of the conventional flowsheet of five, and it out performs the capital cost and energy requirements of the original flowsheet. The example illustrates that any form of sequence selection and energy integration of the original flowsheet is surpassed by the simplification effort as applied.

Extraction followed by a distillation separations is another opportunity for improvement. The boiling points of the five components involved are shown, together with equilibrium coefficients of the components A, B and P versus the solvent, in Figure 4.21. It should be said that component B forms an homogeneous azeotrope with product P. In this example it is decided to break the azeotrope with an extraction. The original separation scheme is presented in Figure 4.22. In this scheme, which consists of four columns, it was decided to extract both components A and B; thus a large extraction column was needed, as component A had a low equilibrium coefficient. The first generation improvement (Figure 4.23) was realized by the installation of a divided wall column in the solvent recovery stream to separate A, B and the solvent. The result was the removal of one column. The next improvement was realized by changing the target separation for the extraction. The extractor was now designed for the separation of B only. This resulted in the split of

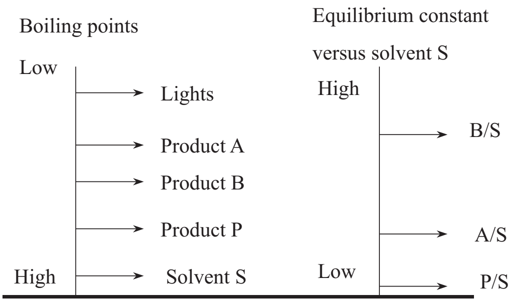


Fig. 4.21. Boiling points and equilibrium constants of extraction example.

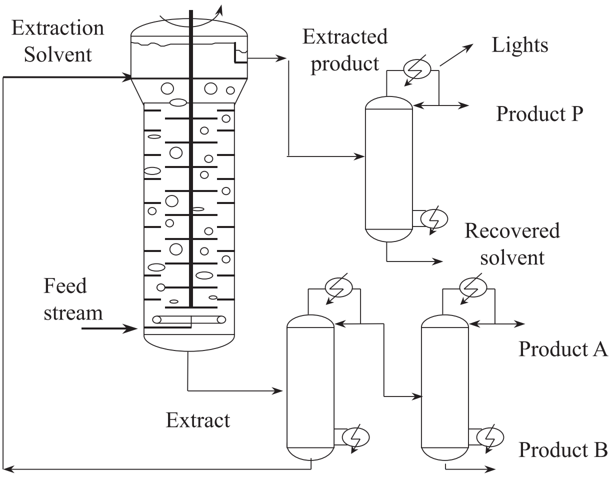


Fig. 4.22. Original extraction concept.

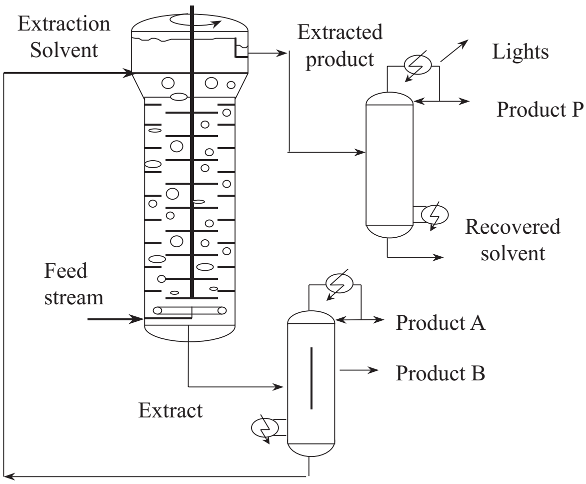


Fig. 4.23. Intermediate solution.

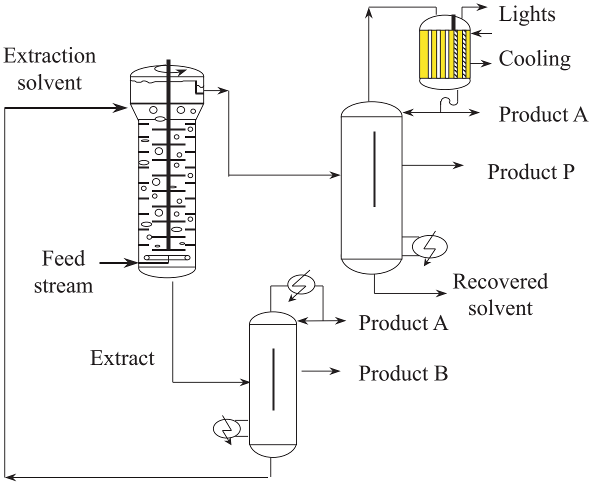


Fig. 4.24. Low cost extraction concept.

component A between the extract stream and the raffinate stream. Product P was now to be separated after the extractor from the solvent, lights and product A. The separation was achieved in a divided wall column. As the lights were closer boiling to A compared to product P, the previous solution of a vent at the reflux drum was not suitable. Therefore, a dephlegmator was installed in the overhead stream of this column. The final solution (Figure 4.24) was much cheaper in capital and energy, particularly as the solvent flow was reduced by a factor of 3, as were the sizes of the extractor and the solvent recovery tower. The dephlegmator was combined with the

Extraction of two components from product stream

The lightest component has a low partition coefficient
The second component has a high partition coefficient and formed an azeotrope with the main product

Original solution; extract both components followed by a distillation

The result was a large extraction column with a high solvent flow

Low cost solution; extraction of second component followed by three component distillation

The result is a small extraction column with lower (1/3) solvent flow, a low cost solution

Fig. 4.25. Summary of extraction example.

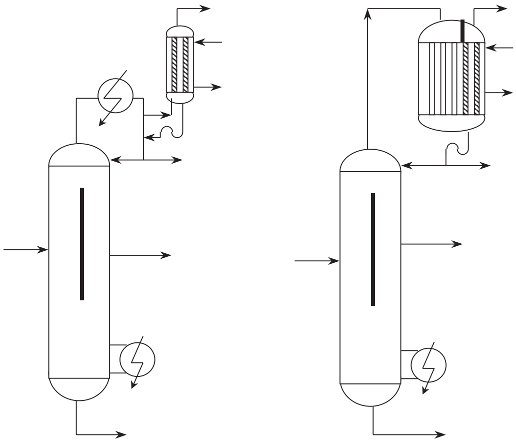


Fig. 4.26. Integration of dephlegmator in the overhead condenser.

condenser of the tower and detailed in Figure 4.25, The combination of a condenser and a dephlegmator or vent condensor an example of a combination of equipment is also applied for other applications as reactor venting, see Figure 5.7. A summary of the above extraction example is given in Figure 4.26.

Note that the simplification examples given here relate only to distillation applications; a more detailed discussion on simplification is provided in Chapter 5.

It is advocated that preliminary sequence selection be exercised during separation step 1. However, careful studies need to be carried out on the integration of separations to simplify the flowsheet before extensive work is performed on final sequence selection and energy integration during synthesis step 2. The simplest solution is not the most economical solution in all cases, although it is the author's opinion that a design should be optimized from a low-cost alternative, and not from an extended flowsheet.

4.2.2.5 **Separation step 2**

The input for the separation synthesis step 2 are the results of the overall synthesis step 1 on reaction separation and integration. The objective is to develop one or two competing flowsheets, these being developed on the basis of the pre-selected sequences of separations. The simplification alternatives [as a result of brainstorming sessions (see **Chapter 10**) and individual clever thinking] need to be involved in the optimization.

Optimization is based on the simulation of selected flowsheet alternatives. Only very definite heat integrations are included, and other options are not exploited at this stage. The energy prices used should be related to the site energy prices as applicable for different energy levels. The flowsheet needs to be robust to enable optimization, and to be divided into sections like reaction and separation to reduce the size of the problem. In Sections 4.1.4 and 4.1.5, it has already been explained how the intermediate prices must be determined and updated for each optimization level. The optimizations are carried out at different levels. The flowsheet description increases in detail (as explained previously) at each higher level of optimization, and the number of alternatives and DOFs are adapted. At this stage (separation step 2) the second layer of optimization is applied. The optimizations are made for each process section based on NPV calculations, with a limited number of DOFs. To perform these optimizations the simulations need to be completed with a cost section and an economic section. The cost functions need to be adapted to avoid any discontinuities. The selected units are not yet heat integrated at this stage. Distillations are described as short-cut models to eliminate any mixed integer problem, and to assure a more robust simulation. The number of DOFs is reduced by setting those conditions which at this stage have limited impact. So, the separation specifications and process conditions as pressure of operation might be fixed arbitrarily.

The best two to three flowsheets with the highest NPV are selected for process integration step 2.

Summary

Separations are, in most cases, an implicit part of the process. In some batch processes the finishing of products (including the separation) is carried out in the reactor vessel, but for a continuous process (as is being discussed here), a separation train is designed.

- The process design of the separation train starts with an input and output stream diagram of the overall process. In the stream diagram it is essential next to the major components, to indicate specifically the impurity formation and its removal. This is particularly important as recycle streams may accumulate impurities in the process, and cause problems. Occasionally, specific purge streams need to be envisaged for impurity removal.

- Selection of separations follows the heuristic rule that heterogeneous separations are preferable, and should be applied before homogeneous separations The choice of phase separations is self-directing, and depend heavily on the particle/droplet sizes
- Homogeneous separations can only be performed by the addition or creation of another phase
- Heuristic rules are given for homogeneous gas and liquid separations. If the selection of separation technique is not clear, there is no alternative for a cost comparison.
- The most often used separation techniques for homogeneous gas and liquid systems are distillatory separations as distillation, absorption, and stripping. These can be easily (and reliably) designed from equilibrium data, while sharp separation is achievable in one unit. The disadvantage is that capital and operational costs are high.
- The generic superstructure for separation (Douglas and Stephanopoulos, 1995) was found to be widely applicable when compared with several industrial processes.
- The pre-selection of distillation sequence during step 1 is generally made by evaluating all alternatives that satisfy the constraints. Evaluation can be based on the criteria of minimum vapor flow.
- Simplification examples were given for separation trains. In one example, a five-column separation train was reduced a two-column concept. This was realized by the installation of divided wall columns and dephlegmator technology. Simplifications represent the integration of functions and units (see **Chapter 5**). Simplification is needed before step 2 of the synthesis work
- Optimization of the separation sequences is performed on full economics during step 2, but with a selected set of DOFs.
- The selection should be limited to two or three flowsheets, which are further developed during process integration step 2.

4.2.3
Process Integration

The final deliverables of process integration (Smith, 1995; IChemE, 1997) are selected flowsheets which due to a higher level of integration are more efficient and major equipment dimensions for the further evaluation of controllability.

Process integration is a development which is aimed at increasing raw material and energy utilization of a design, and was initially driven by the energy crisis of the 1970s. Nowadays, these are even further intensified and seen to be much broader by the need to create a sustainable world, mainly by further reduction of the consumption of natural resources. Process integration may lead to complex operations which require careful design. We can differentiate process integration as:

- integration *within* a process (section);
- integration *between* specific processes; and
- integration at *site level*.

Another differentiation can be made by splitting the streams into the functions which they perform; thus, we may differentiate between:

- Raw material streams; raw materials are in general totally consumed and often depend on a single source supplier.
- Utility streams, such as energy - power and heat-, process water, cooling water, refrigeration, fuel, nitrogen etc.; these might be obtained from suppliers, and can be rated in quality terms (voltage, purity, temperature/pressure level). These streams might be consumed like fuel and power or pass the process and are exported at another purity or energy level.

The constraints – which are clearly an important part of integration – will be discussed initially, after which specific aspects of integration with raw material and utility streams will be detailed. An overview of trends and developments in process integration has been presented by Gundersen (1999).

4.2.3.1 **Constraints**

There is a strong drive to integrate all kind of streams in order to improve the designs. Limited attention is given to the constraints, which are inherently coupled to integration. From a design perspective, while all stream are considered constant, in actuality they are subject to *availability*, *variability*, and *disturbances*.

Violation of the constraints will not be dramatic, but will result in penalties that manifest as production loss or quality of operation.

It is essential that different aspects of constraints are recognized:

- Dependent or independent operation of a process (section)
- Operability
- Controllability
- Safety and environmental
- Economical

Dependent or independent operation of a process This is a choice that must be made. The initial operational remarks should be made about the level of integration, as integration within a process requires careful consideration of the operational strategy. Is the process operated as one train, or is it divided in sections? A process is often designed to have logically identifiable sections, and a division in operational sections always includes some intermediate provisions between sections. In the example of 1-octene the different operational split can be made between the telomerization, hydrogenation, and ether cleavage (see Figure 4.2). We may create three, two, or one independent operable section(s) in this situation. With two independent sections the choice might be to couple the telomerization and hydrogenation as one operational section, or to couple the hydrogenation with the ether cleavage as one operational section. Similar situations occur when there is a one-by-one situation between a supplier plant and a receiver plant – direct integration between plants. Examples are a single oxygen plant coupled to ethylene oxide plant, or a hydrogen plant coupled to a hydrogenation process. In all these case the decision must be made whether to operate as one unit without intermediate storage, or to install intermediate storage. These decisions can be supported by quantified information about process reliability and availability, with the cost of interruptions versus inventory cost (see **Chapter 7**). Simple and robust plants opt for minimizing inventory by improving plant robustness, but realistic calculations are needed to guide the decision making.

When a decision has been made to operate as one section, then direct integration is applied, although adequate provision is required to obtain robust operation and control. This last situation is often applied between an exothermic reaction section and finishing section where the heat is applied for separation.

In case the decision is to operate sections independently, then the integration between sections needs to have some back-up provisions. This might be from an independent source (as provided by utility systems), from a second source (as in coupled hydrogen supply systems), or from an inventory system (Figure 4.27). These decisions might be supported by reliability and vulnerability calculations. Options for integration at utility levels are illustrated in Figure 4.28. Three alternatives for integration are shown: direct coupled; coupled with internal back-up; and external utility back-up.

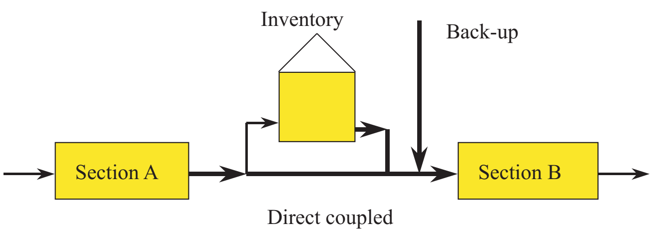


Fig. 4.27. Integration options between processes or sections: direct coupled, through storage, with back-up.

In order to optimize the design, a good insight into reliability and the availability of supplies is essential, both internal and external. Bear in mind that over-demanding guarantees in this respect will be a disadvantage for the receiver – it all boils down to a problem of optimization. Guarantees have a price ticket that is ultimately paid by the customer. The reliability and availability of utility and raw-material supplies and site vulnerability will be discussed in **Chapter 7**.

To summarize, process integration is a development by which the efficiency (raw material and energy utilization) of an operation may be increased, the options for such integration being: direct coupled; coupling through inventory; or with a back-up supply. The constraints that occur are in availability, variability and disturbances while violation will result in loss of production and/or a poorer quality operation.

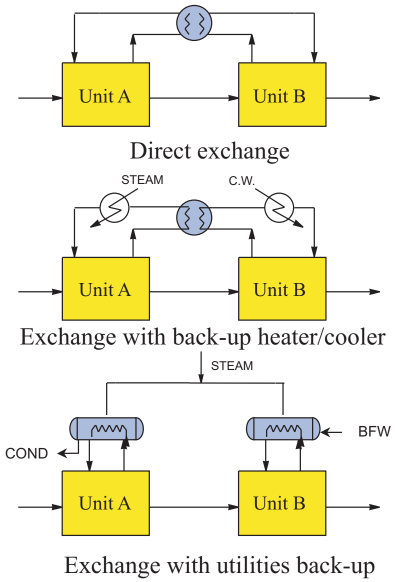


Fig. 4.28. Heat exchange options between process units.

Operability The points for consideration regarding operability are important, as these may lead to additional provisions that require more capital. One questions to be addressed is: Can we cope with sufficient operational flexibility from the consumer, as well as the supplier, perspective? Operational scenarios to be considered are:

- Start-up
- Shut down
- Hot stand-by situation (idle operation)
- Regeneration
- Difference in operational capacities of consumer versus supplier plants
- Difference in operational efficiency compared to design (start-of-run or end-of-run conditions of reactor systems).

The design must be able to cope with these variable conditions in order to permit operational flexibility.

Controllability Next to the availability and variability, disturbances often also lead to problems, and the integration of processes often leads to fluctuations during operation. These may be caused by process variations (disturbances) that are transferred from one section to another, and/or the large response times that are inherently part of integration. The disturbance sensitivity can be identified when static and dynamic controllability studies are performed. Based on the controllability studies, the control strategy eventually including process design modifications needs to be developed to absorb/reject these disturbances. The design of control strategies is an efficient

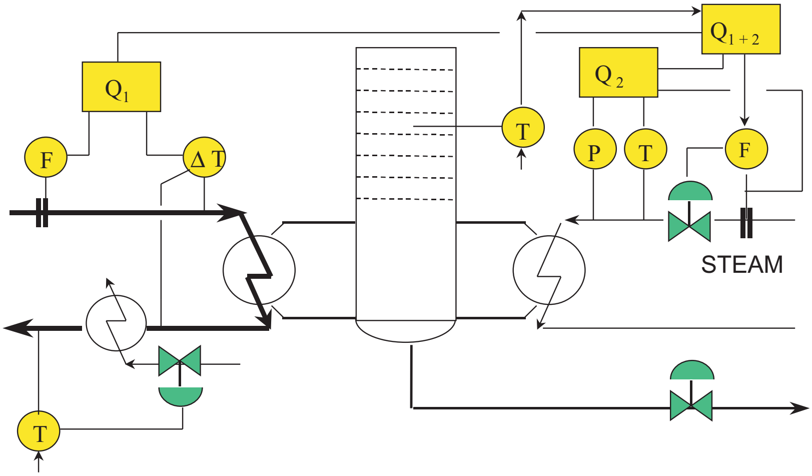


Fig. 4.29. Heat integration between processes with a control configuration to absorb disturbances by heat balance control.

way to deal with these disturbances, and immediate compensation for the disturbances and de-coupling of interactions are ways to do this. Figure 4.29 shows an example of compensation for disturbances for heat exchange between two sections. The subject of controllability analysis is discussed in detail in **Chapter 8**.

Safety and environmental In Section 4.1.2, constraints were discussed from safety and environmental points of view. Although HAZOP studies will draw attention to these problems, they do so far too late in the design, and there will be a need for add-on provisions. Particular attention must be given to streams that are directly coupled with other processes, as any upset may lead to serious problems – perhaps unexpected impurities, a major change in pH, or an oil layer on water (or vice versa). Special attention must be paid to heat-exchanging streams, as these have a tendency to leak over time, potentially leading to problems of inter-reactivity between streams. Special consideration must also be given to temperature-sensitive materials, particularly under low- or no-flow conditions in heaters, as steam control valves always leak and may cause problems of inter-reactivity or plugging. Unexpected situations may also occur with regard to environmental problems.

In conclusion, it might be said that concern exists regarding inter-process connections as a result of integration between processes. Potentially serious problems that may occur during upsets are not limited to direct connections but also indirectly in heat exchangers. In this respect, the design should be driven especially by inherently safer conditions.

Economical Economical constraints speak for themselves, although often there is a tendency not to take the full cost and realistic savings in consideration. The cost of provisions for back-up, controllability, and operability are often not (or are insufficiently) included. The savings are based on realistic expectations (which are seldom at 100% capacity) and the highest energy prices.

The constraints as listed above are a primary condition for clever process integration. In particular, the operability and controllability of the operation – next to safety aspects – are the major preconditions for these inter-process connections and need to be included in the economics..

4.2.3.2 Integration of raw materials

The objective of inter-process integration is to achieve lower consumption of natural resources, and this effort will continue to receive growing attention in light of the sustainability of the environment. Indeed, this is one of the main drivers in the building of integrated complexes. In the past, it has been the reduction in logistic costs which has led to the integration of processes, with resultant large complexes. This drive is now strengthened by a tendency to process less-purified streams between plants in order to save on separation costs. Information on this subject has been published to a limited extent, but has largely been targeted at specific applications.

It was Netzer (1997) who first drew broader attention to these opportunities, and current practice is clearly evolving in that direction. The potential applications of inter-process integration include:

- Streams that require large amounts of energy and capital to separate them from components with similar properties – propylene and propane, or ethylene and ethane separations are good examples. The application of less-purified olefin streams is found in the alkylation of benzene to produce cumene and ethyl benzene. In these applications the receiving plants remove the olefins and concentrate the alkanes; the concentrated streams are then re-sent to the supplier olefin plant as valuable feed.
- When the receiving plant dilutes the raw material stream which has been concentrated at the supplier plant. Examples are hydrolysis processes which receive dried, raw material such as ethylene/propylene oxide, while the stream is diluted again during hydrolysis. Other examples include the drying of monomer streams before use in a watery emulsion polymerization reactions.
- Cooling or condensation of a stream before delivery, while the receiving plants re-heats the stream before usage.
- More interconnections will be created to achieve higher-efficiency operations, an example being the integration of an ethyl benzene plant within an olefin plant (Netzer, 1999).

The opportunities are at hand, particularly as there is a trend to produce chemicals at complexes in order to minimize logistics costs. The above examples can be extended, and most applications have been explored during revamping of processes to find cheap solutions. The trend towards further process integration is clear.

A number of specific problems areas may be encountered with respect to impurities:

- The accumulation of trace components in the receiving process; an overall balance needs to be made to track the removal or destruction of these components.
- The effect of trace components on the reaction of the receiving plant–catalyst poisoning may in particular be a concern.
- Fouling caused by impurities need to be verified before final selection.

Although the constraints and potential problem areas outlined here must be examined carefully before a decision is made, the potential for the development of more efficient processes is clear. As mentioned previously, while consideration of the constraints is primary in the achievement of clever integration, the integration of raw materials evolves automatically in line with site integration (see **Chapter 7**).

4.2.3.3 Integration with utility streams

Utility streams are streams that serve as aids for the operation, for example power steam nitrogen. They are quite commonly supplied by a utility plant either internally or externally, have connections between the plants over the site, and are often rated in terms of quality (purity and temperature/pressure level). For thermal energy these quality ratings can be expressed as a capability to generate work, or also expressed as exergy next to temperature or pressure level for steam. For specific material flows such as water and hydrogen, the quality is expressed in purity terms. These streams are capable of performing a function at a certain level, and might be reused several times at decreasing quality levels. The most exploited stream function is heat, which cascades down by reuse in a process at lower temperature. Energy in the form of fuel might generate power with a gas turbine, and in turn generate high-pressure steam with a boiler unit. The heat then cascades through different energy exchange steps (which generally includes steam turbines and process heaters) until it ends up in the environment. The same applies to specific material streams that are used at high purity, but may be reused at a lower purity level. This technique has been in use for several years, and has resulted in the development of higher efficiency designs. The technique to support these designs is known as "pinch technology/analysis", and this – together with exergy analysis to obtain more efficient process designs – will be outlined in the next section.

Pinch technology Pinch technology was first extensively described in *A User Guide on Process Integration for the Efficient Use of Energy* (IChemE, 1997; originally 1982), and has been captured in a number of different software programs. Pinch analysis is used to address the integration of heat and other service streams.

The principle will be explained below in rudimentary form for heat integration. A temperature–enthalpy (T–H) diagram is made for the process streams to be cooled (hot streams), and the process streams to be heated (cold streams). The T–H curves (known as "composite curves") are an accumulation of the hot and cold process streams (Figure 4.30).

By shifting the cold stream to the left, the composite curves will approach each other until there is a defined minimum temperature difference ΔT_{min} between the

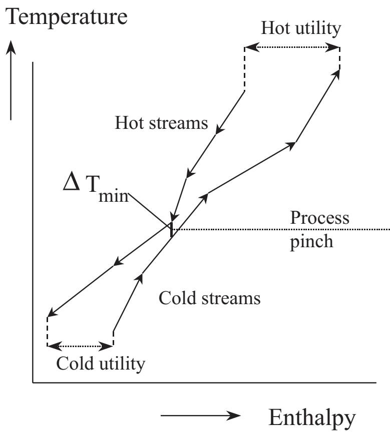


Fig. 4.30. Composite curves.

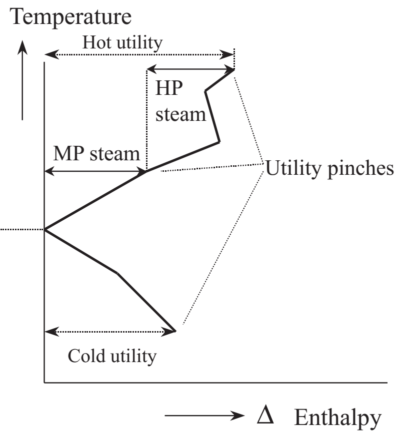


Fig. 4.31. Grand composite curve.

curves. This temperature difference is determined by economics. The point where the composite curves come closest is called the "process pinch point". The composite curves represent the opportunity to exchange heat between the hot and cold streams. The minimum heat to be added, and the minimum heat to be removed, is shown in the same diagram, called the "hot and cold utility". These are the achievable energy targets for the process. The defined temperature difference at the pinch is subject to a trade-off between capital and energy savings. From the set of composite curves a grand composite curve can be drawn which is a plot of temperature versus the delta enthalpy (T–ΔH) of the composite curves. The temperature scale is a shifted temperature. The hot streams are $\Delta T_{min}/2$ shifted colder, while the cold streams are shifted $\Delta T_{min}/2$ hotter (see Figure 4.31).

The following guiding principles have been derived from the (grand)composite curves:

- Heat addition should be done above the pinch, and heat removal below the pinch.
- The minimum energy or energy targets supplied and removed can be derived from the composite curves.
- To achieve the energy targets, heat should not be transferred across the pinch. If heat is transferred from above the pinch to below the pinch, the energy consumption of the system goes up from the minimum amount with the amount transferred: $Q_{actual} = Q_{min} + Q_{transferred}$ (this means that multi-effect evaporators crossing a pinch are not optimal).
- The energy targets can only be changed (reduced) by changing process conditions.
- Utility levels required can be drawn in the grand composite curves now utility pinches are shown.

- A decrease in utility requirement can be realized by the application of the so called Plus/Minus principle by:
  - An increase the total hot stream heat duty above the pinch
  - A decrease the total cold stream heat duty above the pinch
  - A decrease the total hot stream heat duty below the pinch
  - An increase the cold stream heat duty below the pinch (Smith, 1995)

Optimization of the process design to result in lower energy targets can be achieved by exploring several design options (Smith and Linnhoff, 1988), including:

- Adapting temperature conditions of the process streams by changing pressure conditions or compositions to enable cross-exchange of process streams around the pinches (utility as well as process pinches). Shift hot streams from below the pinch to above the pinch, and shift cold streams from above the pinch to below the pinch.
- Energy system guidelines:
  - Placement of heat pumps, including refrigeration cycles, across a pinch.
  - Consider that multi-level cooling, like multi-level heating, is applied.
  - Maximize power generation by installation of a gas turbine in front of a furnace or fired boiler or recovering power at pressure let down stations.
  - Placement of absorption cooling across a utility pinch but the applied heat source should low level heat from below the process pinch. Comparison of an absorption and compression refrigeration systems in a grand composite curve are shown in Figure 4.32, illustrated with permission of IChemE 1997.

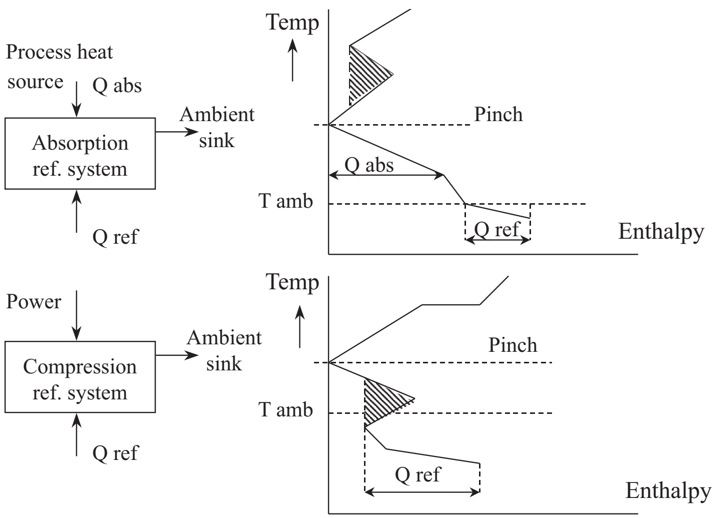


Fig. 4.32. Comparison of an absorption and compressor refrigeration system in a grand composite curve (IChemE 1997).

– Placement of heat engines above the pinch and selection of the preferred utility levels. (Integration of heat engines across the pinch are counter-productive, as heat is transferred across the pinch.)

Care must be taken, as excess heat produced by steam engines at a certain steam level (due to decreasing efficiencies) will be counter-productive, especially if it results in excess at the lowest level and crosses the pinch.

- Reactor conditions are often dominant to integration due to its impact on selectivity, conversion, and catalyst lifetime, if the options are available:
– Exothermic reactors are preferably placed above the pinch.
– Endothermic reactors are preferably placed below the pinch.
– Appropriately designed exothermic reactor sections/processes are, in principle, energy exporters.
– The location of the pinch point is subject to process modification and is not a fixed point during the evaluation of several flowsheet options.
- Distillation separations are preferably not across the pinch:
– Manipulation of distillation conditions to improve heat integration are legion (see Figure 4.33).
– Double-effect distillation is effective if one column is placed above the pinch, and the other below the pinch.
– Installation of side reboilers should be above the pinch.
– Consider partial condensers instead of total condensers in the overhead distillation column, and feed vapor to the next column (see Figures 5.32 and 5.33).
– Vapor recompression is only attractive at small temperature differences and across the pinch (see "heat pumps")
- Evaporators (multi-stage) should preferably not be across the pinch:
– Multiple stages reduce the transfer of heat across the pinch, but this is not the ultimate solution.

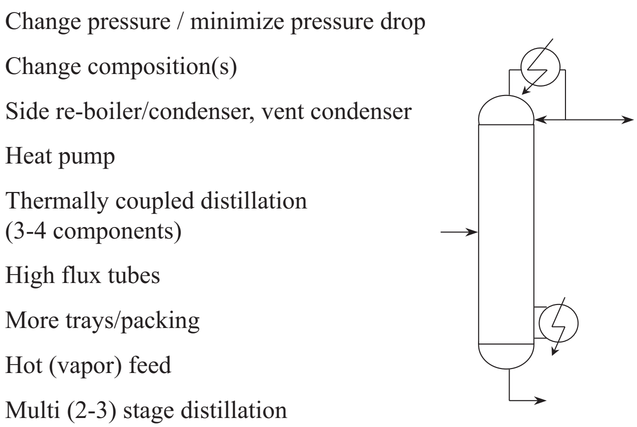


Fig. 4.33. Opportunities to modify distillation columns to realize savings (internal and external).

– A split into stages above and below the pinch which are not thermally linked, or into two parallel staged systems, might be favorable.
– The ultimate simple evaporator is a one-stage evaporator below the pinch, and driven by excess heat, or above the pinch where the overhead heat is used for other applications (this is not this a simple design).
- Generic points
– The minimum number of heat exchangers to be installed is:N min units = (Streams above pinch – 1) + (Streams below pinch – 1)
– The pinch technology is also effectively applied for the development of site energy system (Dhole and Linnhoff, 1992) (see also **Chapter 7**).

Pinch analysis is also applied to other service streams such as water and hydrogen, while the technology is further extended to mass exchanger networks.

The water pinch analysis is based on the quality term expressed in impurity level, and the quantity aspect expressed in mass flow (Wang and Smith, 1994). These analyses received attention as water consumption goes hand in hand with waste water production – which is not appreciated environmentally. The technique determines water flow targets, and shows the effect of regeneration for reuse and recycle to minimize water consumption and waste water flows. In refineries the technique is also applied to hydrogen, as this is a critical component due to its limited availability.

Exergy analysis This is another technique used to optimize design (Kotas, 1995). While pinch analysis was developed to support the development of heat integration in process plants, exergy analysis addresses the overall energy efficiency to minimize energy targets through identification and minimization of exergy losses. The quality of energy is expressed in exergy, which is the maximum amount of work that can be obtained from a given form of energy using the environmental parameters as the reference state. Different forms of energy to be recognized are:

- Ordered energy
- Disordered energy

Ordered energy includes potential, kinetic, and electrical energy, and is fully convertible to other forms of ordered energy, such as shaft work. Examples are hydraulic power converted into electric power, which in turn is converted into mechanical power for lifting a weight, or any other mechanical activity. These conversions of energy can, in principle, be performed at 100% efficiency, although in practice some losses will occur

Disordered energy includes thermal energy and chemical energy. Thermal energy can be converted to work to the maximum with the Carnot cycle, the maximum achievable efficiency

being $\eta_{carnot} = \frac{T_h - T_0}{T_h}$

where T_h is high inlet temperature in °K, and T_o is the outlet temperature of the Carnot cycle.

The maximum conversion of disordered energy to ordered energy (work) is only achieved in fully reversible processes.

Exergy is defined as maximum work which can be obtained from a given form of energy using the environmental parameters as the reference state. (Kotas, 1995).

Exergy is formulated thermodynamically as:

$E_x = (H - H_0) - T_0 (S - S_0)$,

where H is enthalpy, S is entropy, and a zero subscript indicates the reference condition.

Exergy for thermal systems can be written as: $E_x = Q \times \frac{T_h - T_0}{T_h}$

Now energy Q can be divided in two terms:

Q = anergy + exergy,

where anergy is that part of the energy Q that cannot be converted into work.

In addition to energy balances being made around thermal processes (which are based on the conservation law of energy), exergy balances can also be made.
The exergy balance is seen as the law of degradation of energy, this being equivalent to the loss of the irretrievable loss of exergy due to all real processes being irreversible (Kotas, 1995).

Exergy loss over a unit is defined as the difference between exergy input and exergy output or,

$E_{in} - E_{out} = E_{loss}$

where any work added or removed to the unit is included in E_{in} and E_{out}.

Exergy efficiency is defined as

$\eta = \frac{E_{out}}{E_{in}}$

The exergy losses may be of several different types:

- Thermal exergy losses E_{TH}, as in a heat exchanger, where a hot stream heats a cold stream up to a certain temperature: the smaller the temperature difference, the less the exergy losses.
- Friction exergy losses due to pressure drop, $E_{\Delta P}$.
- Heat losses to the environment, which always include an exergy term when a heat exchanger is considered E_{HL}.

It is these exergy losses which require attention for improvements.

The exergy losses over a counter-flow heat exchanger are (Figure 4.34):

$E_{A1} - E_{A2} = \Delta E_A$

$E_{B4} - E_{B3} = \Delta E_B$

$\Delta E_A - \Delta E_B = E_{loss}$

$E_{loss} = E_{TH} + E_{\Delta P} + E_{HL}$

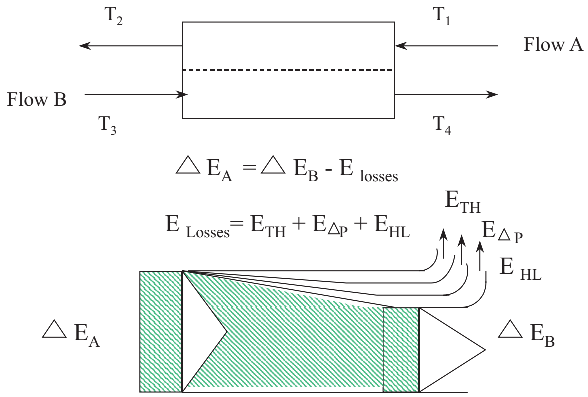


Fig. 4.34. Countercurrent flow heat exchanger with an exergy flow diagram showing the exergy streams including losses.

Flowsheets can be analyzed for exergy losses per unit and represented in a so-called Grassmann diagram which is an adaptation of the Sankey diagram used for energy transfers. Flowsheets are capable of making an energy and exergy balance (Hinderink et al., 1996). The exergy flow diagram, also called Grassmann diagram, shows not only the losses but also splitting of exergy streams, as well as the recirculation of exergy. A good example is a gas turbine cycle provided with a air preheating where the exergy flow diagram makes the recycle of exergy flows and losses clearly visible, see Figure 4.35.

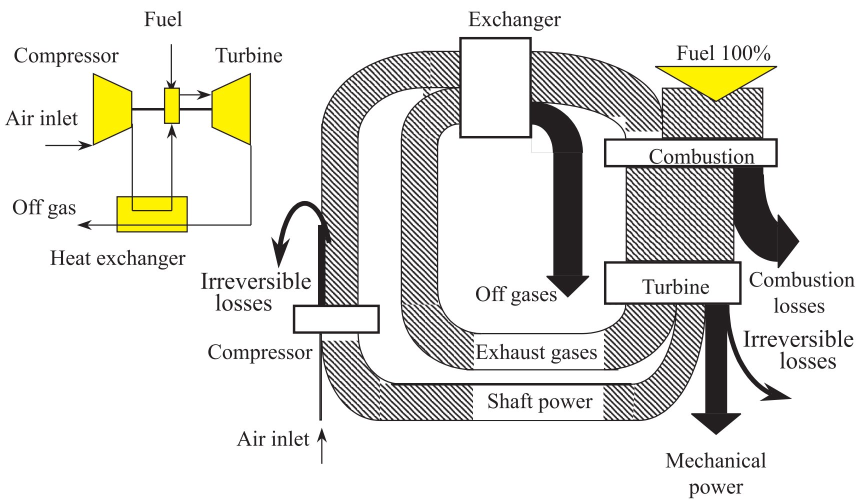


Fig. 4.35. Exergy flow diagram of a gasturbine cycle with air pre-heater.

Exergy analysis provides a good insight of where exergy is lost, the losses often being caused by:

- combustion of fuel, conversion of chemical energy to thermal energy during combustion with air results in a large exergy losses:
- a large temperature difference between streams, as in furnaces or boilers where the flue gas temperature is much higher than the cold stream;
- friction, as in throttling valves or piping;
- efficiency term in turbo machinery;
- mixing of streams at different concentrations and or temperatures; and
- separation efficiencies (low number of effective stages).

The following example shows alternative ways of minimizing exergy losses in a fired reboiler (Figures 4.36 and 4.37) (Note that a steep temperature curve in the bottom of the reactor would favor a solution). The following opportunities can be exploited:

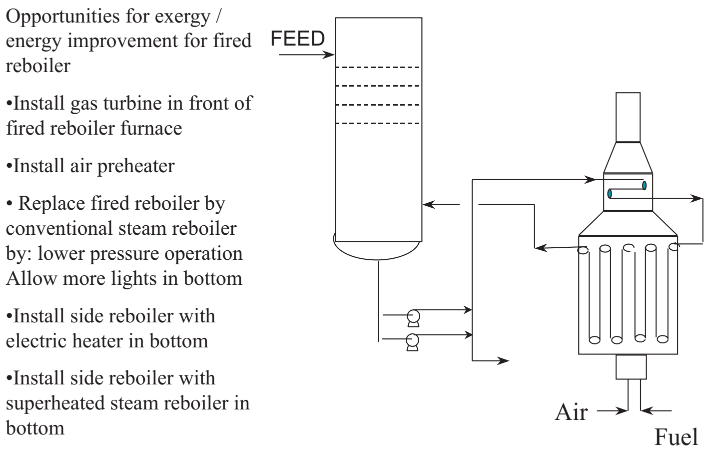


Fig. 4.36. Alternative options for a fired reboiler to save energy.

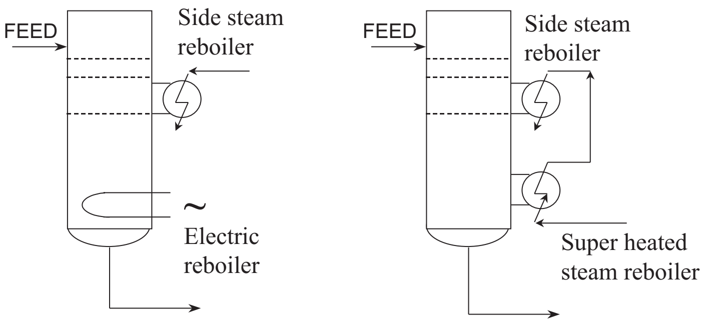


Fig. 4.37. Side reboiler complemented with electrical heater or superheated steam heater as bottom reboiler.

- Install a gas turbine for power generation in front of the furnace.
- Install an air pre-heater at the furnace.
- Replace the furnace by a steam reboiler through evaluation of the following alternatives:
  - Lower pressure operation *in the bottom* by ensuring less pressure drop over the column and/or a lower top pressure.
  - Allow more lights *in the bottom*.
  - Install a side reboiler and utilize the superheat of steam for *bottom* heating.
  - Install a side reboiler and utilize an electric heater for *bottom* heating.

Temperature and pressure and concentration profile On occasion, designers prefer to make a profile of different conditions flowing through the process. (Grievink). Normally, the conditions monitored are those of pressure, temperature, and concentration, plotting of which renders visible how often there are "jumps" in processing of the material. In particular, *"do", "undo" and "redo"* situations are made visible. These plots are made only rarely, but clearly help to identify improvements.

In conclusion, pinch and exergy analysis are complementing tools with which the engineer can analyze and improve the energy situation. The challenge is to develop ideas to minimize energy consumption by:

- identification of opportunities for minimization of energy targets by exergy analysis;
- energy integration supported by pinch analysis.

Although the tools show targets and losses, the creativity for improvements must originate from the engineer.

4.2.3.4 The design of an energy structure

The development of an energy structure around a process is subject to a certain strategy. A basic approach consists of the following sequential steps:

1. Divide the process into independent operational sections and take care of back-up provisions for input and output streams of an independent operational section
2. Develop the constraints for integration (as discussed in Section 4.2.3.1).
3. Analyze the process with exergy and pinch techniques and explore options for process improvements. This might be time-consuming, but it is worthwhile. Process integration carried out after the process streams have been fixed has limited impact compared with process modifications. The results of the improvements are reflected in lower targets.
4. Develop a preliminary process energy structure in relation to the site energy structure selection of levels of exchange on steam temperature and pressure, drivers (electrical versus steam) and generation of steam and power, (Townsend and Linnhoff, 1983). Basically the site utility levels are the first choice for reasons of back-up and exchange between processes, **Chapter 7**. In case pro-

cess heat can be generated at a steam level between the utility levels, for usage at another plant section a plant intermediate steam level might be appropriate.

5. Develop a plant energy system which is largely independent from external steam supply, without violating the benefits of site integration. This to reduce its vulnerability, the transfer of large amounts of steam across the site and its related dynamic effects.
6. For network integration, the following implementation rules need to be applied:
   – Apply process integration in the following order of priority: unit, section, process, site (complex).
   – Apply heat exchange between flows of similar heat capacity (mass flow × specific heat, $M \times C_p$) are preferred, rule of Gommers.

   The inlet and outlet streams of reactor systems are often counter currently crossed as well as the inlet and outlet of a furnace (air pre-heater with flue gas). Another example is the exchange between solvent streams of inlet and outlet of absorber/desorber. The above examples comply with the integration per unit/section, and will also give close to parallel temperature profiles which lead to limited number of exchangers.
   – Apply process simplification in relation to process integration, avoid process stream splitting unless operability and controllability problems are adequately solved while saving are considerable.
7. Develop a strategy for drivers in the process (electrical versus steam versus gas turbine, which fit in the site infrastructure). The desire to avoid a common cause failure is a point for consideration

The above approach is applied during process integration 1, and upgraded at step 2. During process integration 1, the preliminary energy structure is developed and the energy values for the different steam levels must be determined as these need to be used for the level 2 reactor and separation synthesis. In step 2, the challenge is to adapt the process conditions to minimize the energy targets before energy integration is applied.

4.2.3.5 **Simplification with integration**

During the development of an energy structure it is important to avoid many cross-connections and ultimately to keep a well-ordered process. This is one of the reasons why operability and controllability were introduced as constraints for integration. The following basic rules are to be applied:

- The application of an order of priority for process integration from unit, section, process and complex is one of the starting points for process simplification.
- The application of heat exchange between flows of similar heat capacity (mass flow × specific heat).

The design philosophy of clever process integration finds its starting point here. In this section, some reference is made to simple design solution that is specific for energy integration.

For reactor systems, simple designs have an integration with the energy structure. When we look at the examples presented under reactor simplification we immediately notice the integration with energy. The example in Figure 4.6 reflects a loop reactor replaced by a boiling reactor where six exchangers are replaced by one exchanger. Any form of energy recovery in this concept is more likely to be performed economically.

When we compare the replacement of three cooled CSTRs with one adiabatic CSTR and an adiabatic plug flow (Figure 4.7), the improvements in reactor configuration are striking (low cost at close to identical selectivity and conversion). The improvements in energy recovery are also significant, as all the reaction heat is now available in the effluent for utilization in the separation section.

The development in nitration technology show a similar effect when cooled CSTRs are replaced by an adiabatic plug flow reactor, while heat utilization is directly applied for separation, Figure 4.8.

The reverse flow reactor (Figure 4.9) includes cross-exchange between reactor inlet and outlet in the reactor vessel, with utilization of reaction heat. More examples are known, but it is these examples that clearly illustrate the usefulness of clever integration of energy and reactor.

The energy structure for an exothermal reactor heat train shown in Figure 4.38 covers the following elements:

- feed effluent exchangers at maximum temperature levels;
- steam generation at utility level exportable to other independent operable sections/processes; and
- start-up heater combined in the steam generator saves a piece of equipment; at high temperature levels, heating could even be realized by utilization of steam superheat.

This concept cannot always be followed – especially not when phase separation is involved. In that case a variant must be introduced.

The energy structure for high-temperature, endothermic reactions is shown in Figure 4.39.

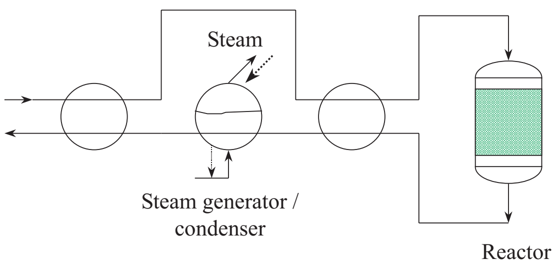


Fig. 4.38. Exothermal reactor with feed effluent exchangers and steam generator for heat removal also operable as heater for start-up by reverse flow operation.

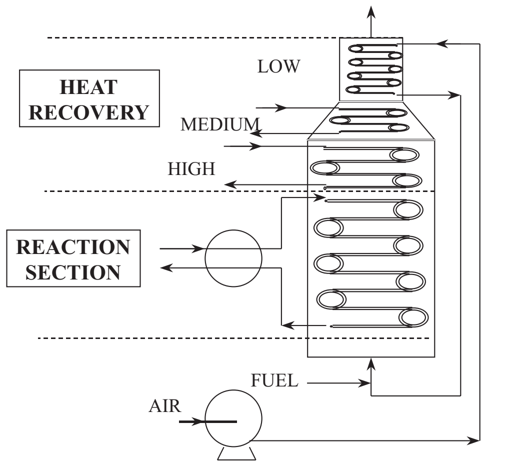


Fig. 4.39. High-temperature endothermic reactor in furnace with heat recovery system.

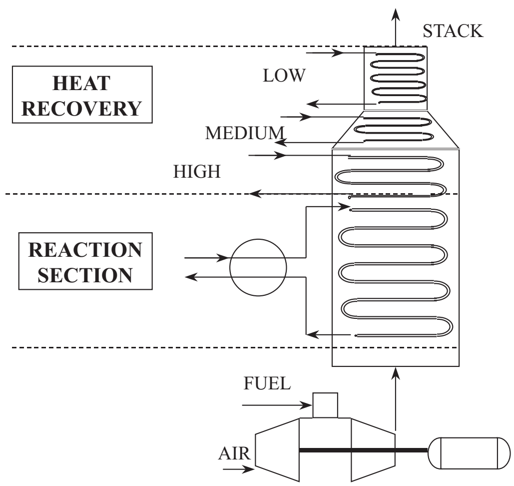


Fig. 4.40. High-temperature endothermic reactor in furnace with gas-turbine and heat recovery.

This structure is characterized by crossing flows of similar heat capacity (mass × sensible heat), and consists of:

- feed effluent heat exchanger for process flows; and
- feed effluent heat exchange of flue-gas with air inlet (air preheat).

In this case the choice is the temperature level of air preheat. In principle, we prefer to preheat to maximal level, as the saving is on primary energy. The constraint is determined economically, as higher temperatures ask for more durable, expensive materials to construct the air pre-heater and radiation sections.

An alternative for this structure is a furnace provided with a gas turbine (Figure 4.40). In this alternative, the process streams are cross-exchanged but the option for air pre-heating is not available. Therefore, the flue-gases must be cooled at decreasing temperature; this is shown as high, medium, and low heat recovery.

For separation systems, we have a similar type of integration effort. The activities to minimize energy targets through flowsheet modification (as shown in the distillation train example; Figures 4.16–4.20), has to be extended by clever energy integration, which is a challenge. The application of an order of priority: unit, section, process, site (complex) is also applicable for separations. One might consider heat integration between an extractive distillation column and the successive solvent from the stripper column. In the case of a large difference in pressure between an absorber and desorber, a reverse-running pump to drive the solvent circulation might also offer a clever integration option.

With the above designs the basic rules for heat integration are reflected.

4.2.3.6 **Is there conflict between process integration and process simplification?**

The target for simplification was to explore options from a simplicity perspective to achieve a high-quality, economical, optimal process. The objective for process integration was to determine minimum consumption levels – to challenge the targets and, based on a minimum target, to design integrated networks that optimize the design.

By following the approach of pinch networking without restrictions, the result might be complicated configurations. Both approaches must respect the constraints as applicable, including operability and controllability requirements. In particular, these requirements will put a damper on unrestricted integration. An integrated process which does not have sufficient disturbance rejection capability will not be exploited to its design intent. The answer to the above question is that, as long as the decisions are based on the most economical solution while respecting the constraints, there should not be a conflict.

Summary

Process integration is an activity that is applied extensively, its initial objective being to reduce energy consumption. Nowadays, the objective is extended to minimize the use of natural resources from the perspective of creating a sustainable world. Process integration may result in complex operations, and therefore requires careful design, with recognition of its limitations.

- Process integration can be differentiated in:
  – Level of process integration; per unit, section, overall process, between different processes and at site level.
  – Streams, as raw material and utility streams.
- Constraints are a major issue during integration, and these need to be analyzed carefully to avoid large disappointments during operation, the factors that play a major role are; *availability, variability and disturbances.*
- Constraints may be notified if we address the following questions:
  – How dependent or independent is the operation of the integrated streams?

- What is the effect on the operability of the process?
- What is the effect on the controllability?
- What is the impact on the safety and environmental aspects?
- Constraints can often been neutralized by adequate provisions. Are these provisions included in the economics?

- Integration of raw material streams at chemical complexes (direct connection between processes) receives growing attention, as economic savings can be considerable.
- Integration of raw materials receives specific value in cases when:
  - lower-purity (below market quality) products can be processed. This often leads to less separation effort at the supplier side; for example, an ethyl benzene process can effectively separate ethylene from ethane during reaction.
  - a product can be delivered in a condition where it effectively can be utilized by the consumer. Why are process streams concentrated or condensed, while the consumer dilutes or evaporates these before usage? The *do, undo, redo* statement is also applicable between processes.
  - the storage of highly toxic materials can be avoided or minimized, e.g., for chlorine.
- Integration of utility streams. Utility streams can be rated in quality terms. For thermal energy, the quality term is its capability to generate work also expressed as exergy, next to temperature and steam level. Other streams such as water and hydrogen are often ranked in purity terms. The quality rating was introduced to enable reuse of a stream by cascading it over several process functions, as is widely applied for integration.
- The technique to minimize usage of utility streams is called "pinch technology/analysis". This was originally developed for energy reduction, after the energy crisis in the 1970s. The method was based on the identification of the minimum amount (target) required for the flowsheet under study, and taught how to approach this target. Pinch technology, meanwhile, has been extended with other service streams such as water and hydrogen.
- Pinch analysis has resulted in the development of design guidelines which have been listed.
- Pinch analysis should not be limited to the process, but also applied to site/complex integration.
- A well-known technique to identify opportunities for improvements is based on exergy analysis. This technique has been described and illustrated with exergy flow diagrams also called. Grassmann diagrams clearly show where exergy losses occur.
- The order of priorities to achieve simple and low-cost (energy-wise) solutions is: *Apply process integration in the following order of: priority; unit, section, process, site (complex).*
  - Another order of priority is:
    Apply heat cross-exchange between flows of similar heat capacity (mass flow times specific heat).

    These two orders of priority do *not* need to be in conflict.

- The contradiction between process integration and process simplification. Pinch analysis, being the bases for process integration, is focused on minimization of utilities, and this may lead to a wildly growing network of exchangers. Process simplification will take advantage of exergy analysis as well as pinch analysis, but will implement these in an order of priority for process integration. The final answer must be found in the economics after the process constraints are respected.

4.2.4
Controllability Analysis

Controllability analysis (Perkins, 1989; Skogestad and Postlethwaite, 1996; Seider et al., 1999; Luyben et al., 1998) is an important technique to achieve robust control, especially for simple and robust plants which were earlier defined as:

An optimal designed safe and reliable plant, operated hands-off at the most economical conditions.

The requirement of hands-off operation is new in respect of conventional designs, as it does not focus only on plant automation. Robust control includes the process being able to track its set points and having good disturbance rejection capability over a wide operating window. In other words, operators are no longer part of a control loop – they become supervisors and determine the overall set-point for the operation.

The demand on control – next to hands-off operation – is higher than in the past due to:

- High requirements on product quality.
- Elimination of intermediate storage as lot tanks, check tanks/hoppers and minimization of storage, (implementation of JIP and TQC).
- High level of process integration.
- Switchability of process conditions for campaign operations (switchability is defined as the ease with which the process can be moved from one stationary point to another).
- Bases for closed loop optimization.

The consequence is that the process design needs to include controllability analysis as part of the synthesis process to assure that adequate control is possible. It was John Perkins, 1989, who specifically draw attention to the interaction between process design and control (For details on controllability, see **Chapter 8**.) At this point, only the overall methodology is discussed.

Controllability analysis is split into two parts:

1. *Static analysis* is executed when the first flowsheet selection is carried out, at the end of synthesis step 1, and is used as input for synthesis step 2. Further static analyses are performed during step 2, when the mass balances of the alternatives for evaluation become available.

2. *Dynamic analysis* already starts parallel to all steps 2, and needs to be completed before the final selection of the process alternatives.

4.2.4.1 **Static analysis**

Static analysis (controllability step 1) requires the mass and energy balances as input for the analysis. The objective is to determine the window where the process can be operated at steady state and the degree of interaction in the process. This can easily be determined by static simulation, as a change in input may appoint to an unsteady situation when the system does not find a new steady state solution. This is important input also for switchability and for operation optimization, as in both situations the objective is to change set points and to bring the process to another steady state conditions.

Process interaction analysis is performed with static simulations. Steady-state gains of the flowsheet and interactions are determined based on the perturbations of the input one at a time. The overall successive steps of the methodology are as follows:

1. The flowsheet must be divided into subsystems, feed system, reactor section, evaporation section, or distillation section, and any sensitive recycle system (sensitive in the sense that it has a reasonable impact on reaction or separation). It is not necessary to select all processing units for an interaction analysis at controllability step 1 – only those that are suspicious for interaction. We know that a distillation column, an extraction, absorber and stripper as single processing units are controllable. An interaction analysis within these last units can be started, but this may be better postponed to controllability step 2.
2. Determine the degree of freedom analysis and, as a result of this, the number of independent variables.
3. For an interaction analysis, the input and output variables must be determined. The output variables are those variables that should be controlled as product qualities, streams, pressures, levels, etc., and these are called the "controlled variables". The input variables are those independent variables that affect the process and its outputs. The input variables are subdivided into manipulated variables (such as valves) and disturbance variables. The number of independent manipulated variables isin general equal to the number of controlled variables. Now, the feasible loop combinations are determined which will be part of the interaction analysis, for details see **Chapter 8.**
4. Relative gain analysis starts with the determination of:

$$\frac{\text{Process gain as seen by a given controller with all other loops open}}{\text{Process gain as seen by a given controller with all other loops closed}}$$

The values are determined based on the perturbations of the input one at time. The results of the analysis are shown in a relative gain array (RGA) essentially a matrix which shows the interaction between input and outputs.

From the RGA the control loops can be selected by pairing the controlled outputs with the manipulated inputs in such a way that the relative gains are positive, and as close as possible to unity (meaning no interaction). When a manipulated variable is paired with a controlled variable (control loop) the DOF is transferred to the set point.

5. The results of the interaction analysis at the end of controllability step 1 are used as input for screening of different flowsheet alternatives. In case an economic interesting design alternative would be excluded based on the interaction analysis results, it could be worthwhile to evaluate possibilities to decouple the interaction. A system which has considerable interaction might be de-coupled easily by simple algebraic equations which can be implemented at the basic control layer, see **Chapter 8**.

4.2.4.2 Dynamic analysis

Dynamic analysis (controllability step 2) runs for a large part of its activities in parallel to reaction/distillation/integration step 2 activities. This concept has been chosen, as the controllability studies are very time-consuming and would cause a delay on the project. During step 2 a reduced set of consolidated flowsheets comes available for controllability analysis, while the process integration alternatives are wider under discussion.

1. The split in process section might be revisited, as the integration might connect units which before were considered separated.
2. At that point, RGA analyses must be repeated and used as input for evaluation of flowsheet alternatives.
3. Dynamic simulations must be made for the selected process sections. These will be based on reduced or short-cut models. Most design models are very detailed, and are less relevant for the dynamics of the process. Often, the reactor model can be simplified by the elimination of certain components, or by converting it to a conversion model. Distillation models can be reduced by using clustered components and trays. Time constants and response times are initially estimated based on hold-up estimates and idealized flow patterns. These will be updated as the result of layer 2 optimizations become available, which include preliminary equipment sizing. In particular, it is the dynamic simulation that is time consuming and which must be started early in order to avoid project delay.
4. Determine the type and level of disturbances that the system is expected to reject / absorb. The prevention of a disturbance requires considerable attention, as these should have a higher priority then rejecting them.
5. Determine dynamic controllability parameters such as: dynamic RGA, condition number, Morari resiliency number, disturbance gain matrix to judge the controllability of the flowsheet (these are parameters described in detail the literature). Low controllability performance should be approached by process design and control design solutions to improve controllability. The purpose of this step is not to design a control configuration, but to judge the controllability and enable the selection of a feasible flowsheet for further design.

Ultimately, the control configuration is selected. The controllers need to be designed, and can be tested in the dynamic simulation. Although this is part of the control design, it is outside the scope of the process synthesis.

4.2.5 Flowsheet Optimization

The input of the optimization is the selected flowsheet after controllability step 2. The objective is to deliver an optimized overall plant design, including all major equipment dimensions and mass–energy balances. The design will be input for basic engineering, to specify equipment, and to develop piping and instrument diagrams and its specifications. The optimization activities have been described under layers three and four of the optimization methodology (see Section 4.1.5). The third layer sets the design, while the fourth layer of optimization confirms the overall design, and particularly the sensitivity of the design for price variability. A deliverable of this layer includes a basis for an operational optimization model to be used for operation optimization.

The optimization is concluding the design as developed during the synthesis steps. Any simplification activity should have been incorporated in the design before this flowsheet optimization is executed. Thus, the quality of the optimization is reliant on:

1. business data (price sets);
2. the quality of the synthesis steps;
3. the accuracy of the model development;
4. the robustness of the models; and
5. DOFs made available for optimization.

The quality of a process is always under evolution through: clever thinking; evolving technology; and business and environmental conditions. The quality of the design is only valid within the assumptions made for the design. However, as these assumptions and conditions will change, monitoring of the quality of the design is important. One way to do this is to search for incremental improvements – this can easily be done with off-line optimization runs where the effect of removal of constraints can be quantified (see **Chapter 10**). Updating of the model is essential to achieve optimal operation optimization and design improvement identifiable.

4.2.6 Logistics and Site Integration

Logistics and site integration are two aspects which have an impact on the process design that may be considerable. The evolution of a batch plant is shown in Figures 1.4–7 in **Chapter 1**. It can be seen that the design evolved from one where most of the handling was included. Nowadays, many of the supplies and services are provided from external suppliers at required conditions.

The following elements are to be considered:

- The design of additive systems
- The option to buy or rent services
- The size and number of storage facilities (if any)
- The integration of the site (complex)

4.2.6.1 **Additives**

Additives are increasingly supplied in dedicated containers and prepared at the supplier, and at the correct mix and concentration. These containers are also used as feed vessels and exchanged as soon as they are empty, thus eliminating the loading and unloading of chemicals, with all the associated safety and environmental risk. It also avoids feed preparation, which often requires the handling and availability of additional chemicals and metering facilities, all of which increases the risk of the facility.

4.2.6.2 **Buy or rent services**

The supply of external process services is another approach taken. These external services are not limited to power and water supply, but also might include other utilities such as steam, cooling water, waste water treatment, refrigeration, industrial gases, as well as "direct" raw material feed streams. These services can be bought based on a long-term contract covering (next to cost) an availability/reliability contract. Such a contract needs to be beneficial for both partners, and should be evaluated carefully as it must represent an economical balance between cost spending by the supplier and potential production losses by the consumer. Any over-investment as a result of high guarantees is a loss which result in higher cost. Current reliability engineering techniques are sufficiently accurate to quantify and optimize the investment in availability/reliability of supplies, see **Chapter 6 and 7**. The services can be generated at site, and remotely monitored and operated by the supplier. The chemical treatment of cooling water might also be contracted out to receive maximum attention from an expert company. The benefits from contracting out these services including equipment are that specialty companies can produce services more cheaply and more reliably as they have multiple units running and can standardize on robust designs.

4.2.6.3 **Storage facilities**

The point for discussion here is the direct supply of raw materials via pipelines versus the installation of storage facilities. Chemical plants are increasingly built in clustered locations (complexes), and this facilitates the direct supply of material, thus minimizing storage and transportation cost and reducing safety risks. When direct supply is not practical, storage facilities must be designed for both raw materials and products. The economic sizing of these facilities which include storage in transport depends on:

- the reliability, size and frequency of the supply system;
- the reliability and unplanned availability of the process; and
- the reliability, size and frequency of the delivery system.

The sizing must be based on a supply chain, including its transportation systems. Details about storage optimization are discussed in **Chapter 7**.

4.2.6.4 Integration of a complex

This is a factor that is exploited to reduce the operational cost of a complex. There is no doubt that an integrated energy system and other process stream integration can generate high savings. The integration however also might result in vulnerability of a complex. The design of a complex was historically based on design strategies – an approach that was developed on scenarios and has led to over-design in redundancy provisions. Nowadays, the integration receives more emphasis, and to achieve a low-cost design a quantified approach must be applied to optimize both the design and the provisions for back-up. With regard to design optimization, sufficient techniques are available to establish a good design. With regard to quantification of the vulnerability, reliability engineering techniques are available and provisions can be judged on their economic contribution.

These techniques need to be applied in order to achieve an optimally designed, safe and reliable complex. The optimization of storage and site integration are discussed in more detail in **Chapter 7**.

Summary

A process mostly fits in an environment of several processes at a site (complex). Simple and robust designs of a complex require careful design of facilities in order to benefit from integration and avoid excess investment and operational costs in redundancy. The example of the evolution of a batch process demonstrated the move from a process designed to do everything within itself, to a design that is largely based on external provisions/services.

- Additives are handled under specified conditions in dedicated containers to be used as feed tanks at the consumer plant; this avoids feed preparation and handling.
- Services are bought externally; these range from (traditionally) power and water up to steam, cooling water, refrigeration, fuel-gas and on-line raw materials. The services need to be designed, based on availability and reliability calculations, to cover the total supply line from supplier to customer in order to avoid any over-design that would result in higher costs.
- The direct supply of raw materials with pipelines is practiced more to reduce inventory, handling, and transportation cost while minimizing safety risk. As a consequence, chemical plants are increasingly built in clustered locations, and this also leads to increased integration between complexes and plants.

- Storage facilities are designed based on the availability and reliability of the total supply chain to minimize the logistic costs.
- Integration of processes on a chemical complex with regard to raw materials and utilities creates significant cost savings. The vulnerability of such a complex requires a balanced investment in redundancy. The degree of redundancy requires a careful evaluation, based on reliability engineering techniques in order to avoid over-design.

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Chapter 5
Process Simplification and Intensification Techniques

5.1
Introduction

In the previous chapters, the emphasis was on the design philosophies and the development of a conceptual design to achieve simple and robust plants. The specific techniques regarding process simplification and process intensification are discussed in this chapter (Koolen, 1998, 1999). These techniques, which lead to a simplification of the overall process, are categorized as follows:

- Avoidance or elimination of process functions
- Combination of process functions
- Integration of equipment
- Intensification of process functions
- Overall process simplification

To explain these terms, process simplification concentrates on the application of existing techniques to reduce the cost of a chemical plant. Process intensification is primarily addressing new technology which is at the development stage or early stage of application to address the same objective. Process intensification concentrates on the improvement and intensifying of process units to reduce the size of chemical plants such as "Higee" and other compact techniques. Both approaches are complementary in reducing the cost of plants. The process intensification information is primarily based on development work presented at three International conferences about Process Intensification for the chemical industry (International Conferences on Process Intensification, 1995, 1997, 1999).

The process simplification and intensification techniques will be illustrated with example. Simplification will also be discussed for specific unit operations where overall priority is given by proposing an increasing order of complexity for design considerations. It should be realized, however, that rising to a higher level of complexity might be justified by functional or economical requirements. The process units and items under discussion will be:

- Reactors
- Distillation and absorption

- Extraction
- Adsorption
- Heat exchange
- Fluid transport
- Piping
- Instruments

The objective of this chapter is to show that simplification/intensification is technically achievable. This may be illustrated by technically analyzing the process functions. The reasons why simplification is so difficult originates not only from the history of design and its evolution, but also on how engineers address the problems encountered.

History has an impact on development engineers, and often forces their thinking along well-known roads. Some may call this conservatism; others would call it proven/solid design. As illustration which can be used is the design of a food process plant which, historically, were built on gravity flow. The raw products were brought to the top floor and the manufacturing process passed gradually downwards through the different units at the different floors, the final stages being conducted at ground floor level for transportation, or in cellars for ultimate storage. A typical examples of this is a brewery. However, when pumping became accepted as a standard unit (this was indeed a breakthrough), gravity flow became to be considered only in very limited cases. Hence, evolution showed an alternative pass which became trendsetting for the next generation of plants.

Sequential thinking is another barrier, though this is often not realized. It is determined by the methodology applied during the design process, though engineers are trained in sequential thinking rather than integrated thinking. The development of a flowsheet is a sequential activity. Following many years of development in process units, functional integration of process units has been applied for only a short time. An exception might be found in energy integration, which was strongly stimulated by the energy crises of the 1970s and 1980s, though integration of energy during flowsheet development has been applied only to some limited degree.

Solving problems in an existing situation results in an attitude that restrict people's thinking. In existing process plants the operational emphasis is often restricted to add-on provisions. The attitude of developing "*what if*" scenarios, to strengthen the safety of an operation, is a very useful tool, and most often leads to add-on provisions. Similar questions are raised during design reviews, which often suffer from the same restrictive thinking.

The effort during design should based more on the prevention and avoidance of problems, as this invariably results in cheaper solutions. As Kletz once declared:

What you do not have can't leak.

From the simple and robust point of view, this could be re-phrased as:

What you do not have can't leak and does not cost anything.

It should be realized that the cost of non-existent equipment emphasizes the following terms: capital, interest, operational cost (operational people, energy nitrogen), maintenance, insurance, land, overheads (emergency, guards, management) – and of course you have to make a profit! Although many engineers try to focus on incremental cost, this is the wrong approach.

It is a challenge for the design of simple and robust processes to overcome these conservative attitudes and to be receptive to simplification/intensification technology.

5.2 Avoidance or Elimination of Process Functions

There are a many functions in a process design which might be challenged as to whether their inclusion is really necessary. The identification of these functions, using a function analysis technique, will be discussed in **Chapter 10**, but at this point only the technical opportunities will be discussed.

5.2.1 Tanks and Vessels

In the illustration of a tank farm in **Chapter 1** (Figure 1.3), it can be seen that six tanks are replaced by two. Initially, *check tanks* (which might also be check silos) are only required if it is assumed that the production process is not operating at specification. This assumption is challenged. Instrument technology and control technology are of such a level that, by using an appropriate predictive model-based control design, the quality at the product stream can meet its specification. This requires some in-process provisions (e.g., internal recycle lines) to cope with any extraordinary disturbances.

Lot tanks/silos are often used to smooth the quality of different batches or campaigns of the same product through blending. These storage mixing facilities can be fully eliminated if the process has an appropriate and reliable instrument and control system and consistent operation practices (automation). The differences in product quality of batch plants are mostly caused by inaccurate measurements of feed quantities. One of the most frequent causes is that flows are metered on volume, rather than mass.

Mixed feed tanks are regularly used in batch plants for feed preparation. These facilities are not justifiable if an adequate direct feed system is designed, or if feeds are delivered in containers at the required composition by the supplier. These mix tanks have a low mixing efficiency, large volumes (which are not to be preferred from a safety perspective), and require a high investment.

Storage facilities such as tanks, silos or warehouses might be reduced in number, or even eliminated. In the example, four tanks are reduced to two. Elimination can be realized by:

- direct feed to customers;
- storage of base products only, and by feeding additives during loading or at the customer; and
- production directly into transportation containers.

Optimal sizing of storage volumes based on probabilities in the overall supply lines, from receipt of the raw material until delivery to the customer, is discussed in **Chapter 7.**

By comparing the batch process in Figures 1.4–1.7 in **Chapter 1**, it is possible to see all the above-mentioned options. In the ultimate concept, all tanks are removed from raw material storage, mix feed tanks, lot tanks and product tanks, while transport containers are added for the product and additives. Elimination of these facilities is not a unique situation; all related equipment is also eliminated, such as pumps, mixing devices and instruments, as well as safety provisions and various operational aspects.

5.2.2
Transport of Fluids

In the case of liquids, the standard solution is to use pumps. However, it should be noted that pumps these might be subject to elimination by using:

- gravity flow; or
- pressure difference

Although these options are well known, they are applied only in limited circumstances. Only in cases of extreme competition between technology suppliers are these options regularly exploited on a competitive basis. Plants such as nitric acid or nitration processes are designed commercially to include a minimum number of pumps. This saves on rotating equipment, contributes to reliability, and also often leads to compact process designs. Gravity flow solutions must utilize all liquid head available, and this drives for shorter lines and compact building. The direct dosing of a neutralizer is a simple example (see Figure 3.7 in **Chapter 3**).

Pressurization of the additive containers can be used to avoid pumps and mixing stations if the additives are delivered at the composition required for the process.

5.2.3
Recovery Systems

These are designed to cope with waste gas and water streams. Such systems might be avoided or greatly reduced either by eliminating the large sources of pollutant(s) or reducing carriers such as nitrogen and water flows (see the visionary document about 21st century plant; Natori and O'Young, 1996). Re-design of the safety provision of a NH_3 storage tank (Figure 3.5 in **Chapter 3**) is a good example of avoiding a release system.

The reduction of carrier streams (e.g., water) can be avoided by the elimination of make-up water and direct steam injection in a process using steam ejectors or steam strippers, or water washing without in-process water recovery. An example of this is where a process has a multi-stage air compressor with interstage cooling; the water condensed is considered as waste, as potentially it might be polluted with oil-seal liquid. This water might represent a good source for make-up water, and as such reduces the waste load.

In general terms, the collecting of all kinds of waste streams for treatment should be avoided. A better approach is to set up internal recycle provisions that are specific to each stream and return these to the process at appropriate points.

5.2.3.1 Do-undo-redo Activities

These are often performed during a process, and might include heating-cooling-reheating. Other examples are pressurizing-de-pressurizing-pressurizing, or separation-mixing-separation. To trace these situations a line diagram can be prepared that shows temperature, pressure, and concentration over the major processing routes, see Section 4.2.3.3 in **Chapter 4**. This representation can easily trigger do-undo-redo situations and offer a challenge for a surge in potential improvement. These activities may be considered for the elimination of equipment such as pumps or exchangers, as well as the elimination of recycle provisions to prevent mixing of streams of different compositions and/or temperature that always lead to a loss in exergy.

5.2.3.2 Single trains and installed spares

Single trains will be discussed under overall process simplification (see 5.6.2). The approach regarding installed spares will be discussed under the topic of reliability in **Chapter 6**.

Separations are often more difficult to avoid, but combination with other separation functions are discussed in Sections 5.3.2 and 5.3.3.

5.3 Combination of Process Functions

The combination of process functions into one unit has been extensively developed during the past few decades of the twentieth century.

The combination of different process steps in batch-operated vessels, for example mixing, reaction, devolatilizing, neutralization, stripping, cooling, crystallization, and feeding additions, is the oldest form of performing process functions in a single piece of equipment. These batch operations are typically found in the food and drug industries, as well as in the fine chemicals industry (see Figure 1.4 in **Chapter 1**). The multi-functional use of equipment does not fall under the banner of "combination of functions", as described later. Although it should be noted that multi-functional use of equipment has its merits, we will discuss here the types of combinations that lead to simpler designs in continuous processes (for a review on multi-functional reactor systems, see Westerterp, 1992).

5.3.1
Reaction

This combination is exploited in mixed ion-exchange beds for water treatment. Another application is in the ethylbenzene dehydrogenation reaction, which is endothermal. In this process – which is an equilibrium reaction – the conversion can be increased by the removal of hydrogen, with such removal being achieved by selective oxidation between the reaction stages. In this case, the oxidation step simultaneously generates heat which is used for heating between the stages.

5.3.1.1 Reactive distillation

Reactive distillation has been in use for quite some time in batch processes, although initially it was not known by this name. *Esterifications* are exothermic equilibrium reactions that produce reaction water. By removing this water in a rectification column or dephlegmator on top of the reactor, see Figure 5.9, it is possible to shift the reaction to completion if the water is the lightest component (an example is the preparation of butyl acetate). The application of an esterification and an etherification in both continuous processes are shown in Figure 5.1. The combination of reaction with the removal of components by distillation is called “reactive distillation”. The reaction might be endothermal or exothermal, homogeneous in the liquid phase, or heterogeneous at a solid catalyst kept under liquid while the liquid is at bubble point.

The most well-known industrial applications of continuous processes are the preparation of the octane boosters ETBE (ethyl-*tert*-butyl ether), MTBE (methyl-*tert*-butyl ether) and TAME (*tert*-amyl-methyl ether) (DeGarmo et al., 1992; Doherty and Buzad, 1992). Other applications, next to etherification, include de-etherifications, esterification (as mentioned above), and alkylation of aromatics.

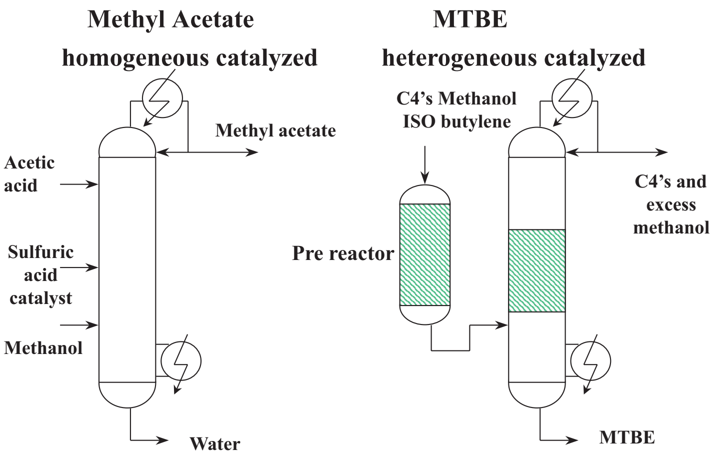


Fig. 5.1. Reactive distillation examples; Methyl acetate and MTBE production.

The application are found in equilibrium reactions, as continued removal of the product(s) shifts the reaction to completion and limits consecutive reactions. At least one product need to be have a higher or lower volatility, which then permits the feeds to achieve product removal by distillation.

The *advantages* of this, compared with the conventional set-up of reaction followed by distillation, include lower energy consumption, higher selectivity, and lower capital cost.

The *limitations* of these systems are equilibrium reactions, reasonable reaction rates at distillation conditions, top and bottom temperatures within operational range, and hold-up in the column for catalyst baskets. Neither feed nor products should inhibit the catalyst, and the reaction kinetics should be available for design.

At low conversion rates, a reaction vessel might be installed at the front of a reactive distillation; alternatively, reaction vessel(s) should be equipped with rectification column(s) or dephlegmator(s)

At high conversion rates, the reaction and distillation are performed in a single column (for an update on reactive distillation and technology, see Schoenmakers, 2000; the development of a synthesizer and designer tool, as part of a European research activity, are also discussed in this article). Modeling has been described elsewhere (Alejski and Duprat, 1996; Zheng et al., 1992; Bollyn and Wright, 1998; Higler et al., 1998), and can be executed in commercial flowsheeting software.

5.3.1.2 **Reactive extrusion**

This is a technique which has been studied for several decades, and which resulted in a number of industrial applications. The understanding of the technology has been developed and reported extensively (Ganzeveld and Janssen, 1993; Ganzeveld et al., 1994; van der Goot and Janssen, 1997; Janssen, 1998). The technology is to be used not only as a tail end reactor but also for co-polymerization reactions in order to obtain new product properties, as applied by large-scale producers of polymers. The smaller-scale polymer industry might apply reactive extrusion to modification reactions in order to achieve specific product properties. The technique is applied to free radical as well as anionic polymerization, examples of which include the polymerization of styrene and styrene-butylmethacrylate, grafting of maleic anhydride onto high-density polyethylene, urethanes, and co-polymerization of methacrylates.

The most important constraints to the application of this technology are reaction time and the reaction enthalpy. The reaction time should be on the order of minutes, as longer time spans will make the process expensive, as the machinery to carry out extrusions are expensive. The preferred adiabatic temperature rise is on the order of 150 °C, while the heat transfer coefficient should be ±400 W/m^2 K. The stability of reactive extrusion has been studied, (Janssen, 1998).

The growing interest in reactive extrusion is based on its capability to operate without solvents yet providing a high conversion. The extruder might be equipped with a stripping section to remove any unreacted monomer. Another advantage is the larger flexibility that an extruder provides compared with conventional reactor systems.

Modeling of these systems has led to extensive progress being made, based on the development of a steady-state reaction extrusion interaction diagram, the reaction kinetics, heat removal, and description of the mixing parameters.

5.3.1.3 Reactive extraction

This is one way to shift the equilibrium of a reaction (Sharma, 1988). This method is also applied to avoid further degradation of a component through in-situ removal. Selection of the solvent is crucial, and not a straightforward task. Next in importance to the distribution coefficients is the solubility in both phases, while the solvent should be inert to the reaction. Some examples reported in literature include:

- the bromination of dialcohols $HO(CH_2)_6OH$ to $HO(CH_2)_6Br$ with aqueous HBr. The problem is to prevent formation of the dibromo product, and this is realized by using a hydrocarbon solvent that forms the basis of a high selectivity. In this specific case, the hydrocarbon extracts the mono bromide and not the di-hydroxy compound, and so prevents the dibromo component being formed.
- the epoxidation of olefinic compounds with the production of metachloroperbenzoic acid in an aqueous phase. This may result in undesirable side reactions, but by introducing the solvent dichloromethane, the product is extracted and thus not available for reaction with the epoxy compound in the aqueous phase. This results in a high yield of the desired product.

5.3.1.4 Reaction with integrated feed effluent exchange

This concept resulted in the development of commercial reverse-flow reactors for the purification of polluted air by catalytic combustion (Matros and Noskov, 1988; see also Figure 4.9 in **Chapter 4**). Catalytic combustion systems are often exposed to a wide variation of the inlet concentration. At low concentration the reaction might starve, while at high inlet concentration the reaction will over-heat the reaction mass. In the conventional design as well as the reverse-flow reactor design provisions have to be made to cope with these situations. The dynamics of the reverse-flow reactors were studied by van de Beld and Westerterp (1996); the synthesis gas production is another application, as described by Blanks et al. (1990).

The main benefits for this technique are capital savings and the resultant very compact units. The limitations are the dynamic understanding of the system which requires dynamic simulations that are capable of handling discrete operations.

The integration between reaction and heat exchange is an option which has been practiced for many years in shell and tube heat exchangers, although in these cases the integrated heat exchanger network designs have often made the system rather complicated from a control perspective.

5.3.1.5 Reactive adsorption

A gas-solid-solid trickle flow reactor for equilibrium reactions was developed to a large extent at the University of Twente in The Netherlands, and was concentrated mainly on the synthesis of methanol (Kuczsynski et al., 1987; Westerterp et al., 1987 and 1989). This is an example of how complete conversion can be achieved by removal of the product, and is equivalent to the reactive distillation technique. The disadvantage is the circulation system that is needed for the solid adsorbent, and as yet this technique has not yet be applied at industrial scale.

5.3.1.6 Reactive absorption

This has been in use for many years for the absorption of SO_3 in water for H_2SO_4 production and NO_x absorption in water for HNO_3 production. The removal processes for CO_2 and H_2S from gases with different reactants has also been practiced for many years. It might be argued whether this process is really a combination of functionality, as this also might be described as a G/L reactor. The removal of CO_2 from flue-gas through a membrane absorber (Feron and Janssen, 1995) also falls into this category.

A combination of the objective functionalities of reactive absorption includes membrane reactors, and these are currently under development (van de Graaf et al., 1999). These reactors focus on equilibrium gas reactions (gases have higher permeation fluxes), where reaction products are removed to achieve high conversions. In essence, they might also be applied for the addition of a reactant to obtain high conversions in equilibrium reactions. Applications of this technique include:

- Hydrogen removal, as in steam reforming, water gas shift reactions, propane dehydrogenation or ethyl benzene dehydrogenation by removal of hydrogen between reaction stages.
- Oxygen addition, as in syngas production and methanol synthesis, as well as the metathesis of propene from ethene and butene.

A summary of the integration of reaction and other process functions is shown in Table 5.1.

Table 5.1. Combination of reaction function with other process functions, and some applications.

Reaction	***Applications(s)***
Reactive distillation	Esterification, Etherification (MTBE)
Reactive extrusion	Co-polymerization
Reactive extraction	Bromination of dialcohols
Reactor integrated exchangers (reverse flow)	Catalytic combustion, Syngas production
Reactive adsorption	Methanol synthesis
Reactive absorption	HNO_3, H_2SO_4 production, sourgas purification
Reaction / reaction	Mixed ion-exchange, ethyl benzene dehydrogenation with inter-stage hydrogen oxidation

5.3.2 Distillation

In this Section, the combination of functions within distillation is concentrated on the separation of three or more product streams. In this respect, refineries have a long tradition in the removal of more product grades from continuous distillation units, such as crude stills. In the petroleum industry, these side streams traditionally had a wide specification range, but today these ranges have been narrowed, this being achieved by side strippers and improved process control. Batch distillations are often also utilized for the separation of multiple components in different process industries. For most applications of continuous distillations in the chemical industry, the objective has been to produce high-purity materials, and therefore more product streams (more than two) were rarely applied, surprisingly enough even when pure streams were not a requirement.

The alternatives for a conventional distillation column for over two product streams are:

- Side streams
- Divided wall column (two columns in one)
- Dephlegmator (rectification and cooling), also known as non-adiabatic rectification.

5.3.2.1 Side streams

These are achieving increasingly wide applications (Figure 5.2). The drawbacks of side streams are that the purity has a wide range, but quality control is not obvious.

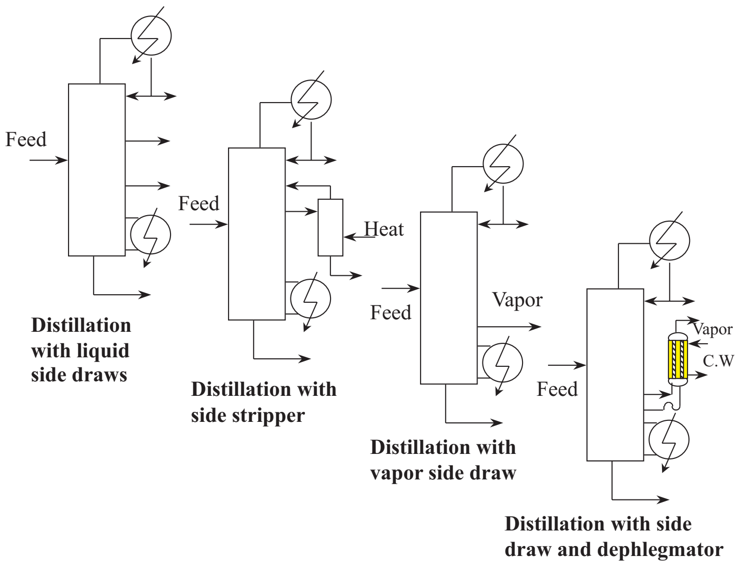


Fig. 5.2. Distillation with side streams.

The increased use of recycle streams in process designs leads to a build-up of impurities. This may lead to control problems on columns, as the traditional temperature measurements for quality control are affected by impurity build-up. The solution is found in the installation of purge streams at selected column locations.

Major product streams can also be taken as a side draw, though one drawback might be that the side stream above the feed point contains lights. A provision with a side stripper, as applied in refineries, might be helpful to achieve a higher enrichment. Liquid side streams below the feed point always contain heavier components. The solution might be found in a vapor side stream to minimize the heavies content in the side stream or further purification of this vapor stream by a dephlegmator (see Figure 5.2, fourth column). A vent stream on the overhead condenser is also to be seen as a side stream. The purification of this vent stream is possible by installing a knock-down vent condenser after the overhead condenser, or by the application of a dephlegmator at the vent. Another applied technique is the installation of a top section on a column (also called a “pasteurization section”) to enrich the vent stream and take the major product as a side stream from the column (Figure 5.3).

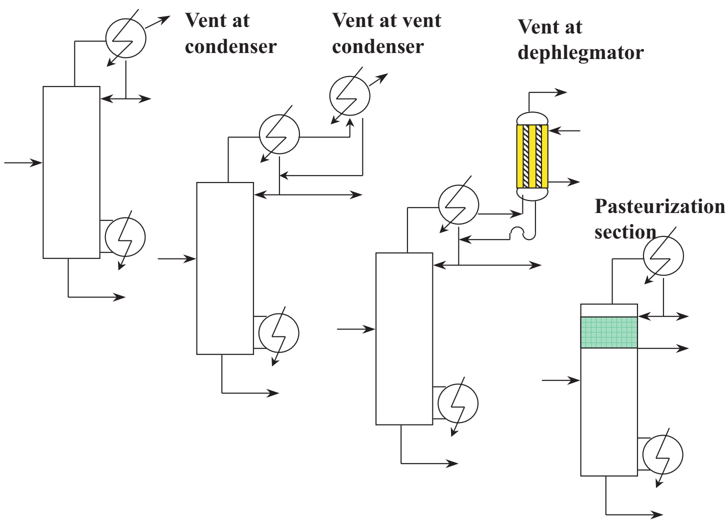


Fig. 5.3. Different vent options for three component separation.

The clear advantage of side draws is that of low cost, while the disadvantages include less purified streams, unless provisions are applied for side stripping or partial condensation of vapor side draws. Adequate control is required, although this would also be a requirement if an additional column were to be installed. The side stripper or rectifier can also be installed inside the column as shown in Figures 5.4 and 5.5, as published by Emmrich et al. of Krupp Uhde 2000.

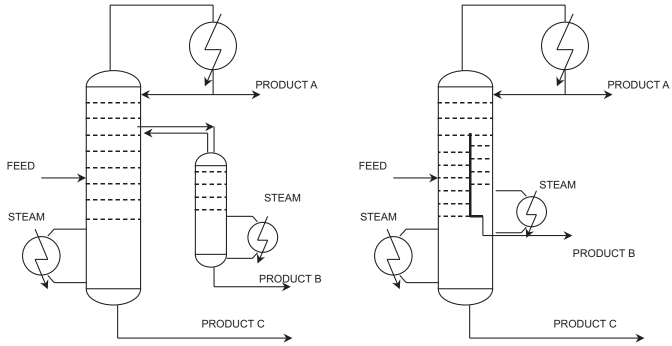


Fig. 5.4. Side stripper installed external or internal (Emmrich et al., with permission of Krupp Uhde).

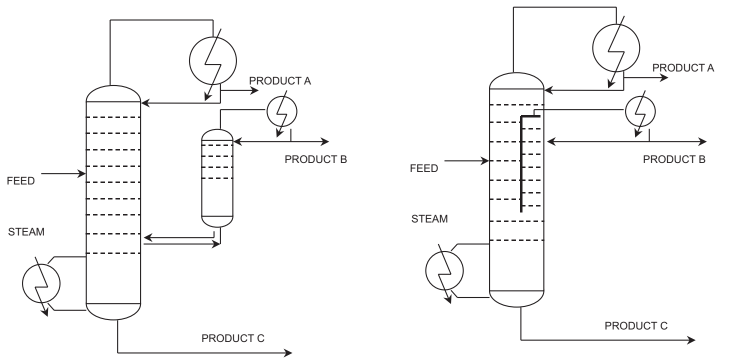


Fig. 5.5. Side rectifier installed external and internal (Emmrich et al., with permission of Krupp Uhde).

5.3.2.2 **Divided wall columns (DWC)**

Divided wall columns are used to separate three to four purified product streams from a feed mixture. This technology, although having been known for decades as the Petlyuk column (Petlyuk et al., 1965), now enjoys only limited application at the industrial scale. The original concept emphasized the thermal coupling between a pre-fractionator and the main column (Figure 5.6). The concept was revitalized by Kaibel (1987, at BASF) through introduction of the divided wall column at industrial scale which emphasized a one-column configuration, resulting in a much cheaper design (Figure 5.7).

The advantage compared with a conventional side draw application is that the system can be designed for any purity requirement. Studies carried out at UMIST in Manchester, UK, have resulted in an improved design and control understanding of this (in principle) rather simple configuration (Triantafafyllou and Smith, 1992; Lestak and Smith, 1993; Mutalib, 1995). In particular, the design of a control config-

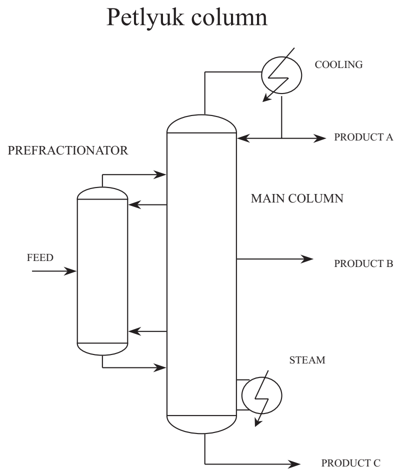


Fig. 5.6. The Petlyuk column, heat integrated with multiple products.

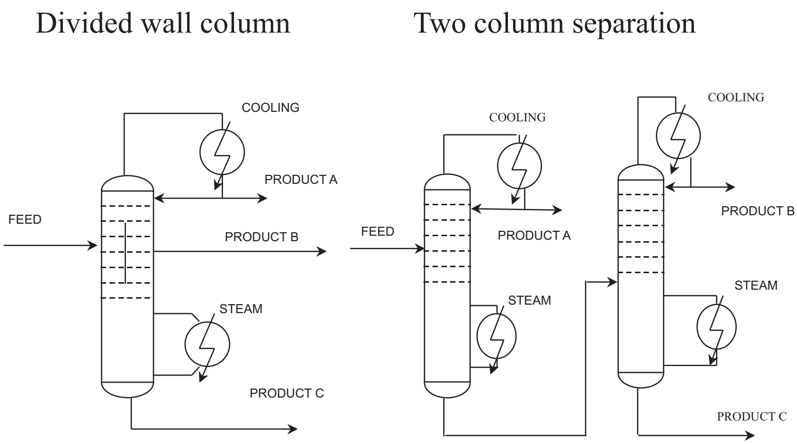


Fig. 5.7. Divided wall column versus conventional two column separation.

uration, which was anticipated as one of the major difficulties, can today easily be designed based on dynamic simulations. Mechanical design problems have been solved, and the uncertainties of control and mechanistics have now been removed. The result has been a major increase in the number of applications – at the time mainly at BASF where the concept was first conceived.

The divided wall columns can realize energy and capital savings of up to 30% compared with a nonintegrated, two-column separation. Moreover, the column can potentially also be applied to four-product separations, though restrictions to such application include:

- differences in boiling point between the light and heavy components, to stay within the normal utility levels for condensing and reboiling; and
- thermal degradation of the products.

Both conditions might force the design towards a two-column set-up operating at different pressure levels.

5.3.2.3 **Dephlegmator**

This is a nonadiabatic rectifier that is designed to operate vertically where a vapor stream flows upward while it is partly condensed. The condensate runs down as a reflux over mass transfer-promoting elements such as trays and/or packing.

During transfer, the vapor stream is purified while the liquid is enriched with the less-volatile components. The device is often designed as a vertical shell and tube heat exchanger provided with cooling, but compact plate fin heat exchangers (PFHE) are also used. There are two options for the design shell and tube exchanger: (i) the process is on the tube side, in which case packing is applied; or (ii) the process is on the shell side, in which case sieve trays are chosen.

An alternative solution, albeit more expensive and complex, would be a rectifying column with an overhead condenser and reflux (Figure 5.8).

For distillation columns, dephlegmators are installed as a vent condenser, or on a side draw (see Figures 5.2 and 5.3). The dephlegmator or partial condenser is also applied at the overhead streams of reactors to cool the reactor and simultaneously remove inert gases (Figure 5.9). In this example, a reflux condenser and a dephlegmator are combined into one piece of equipment. The design aspects of a dephlegmator have been discussed by Jibb and Drögemüller (1999).

The *advantages* of dephlegmators are capital cost reduction and energy savings, as they are thermodynamically efficient since less heat has to be removed to achieve a

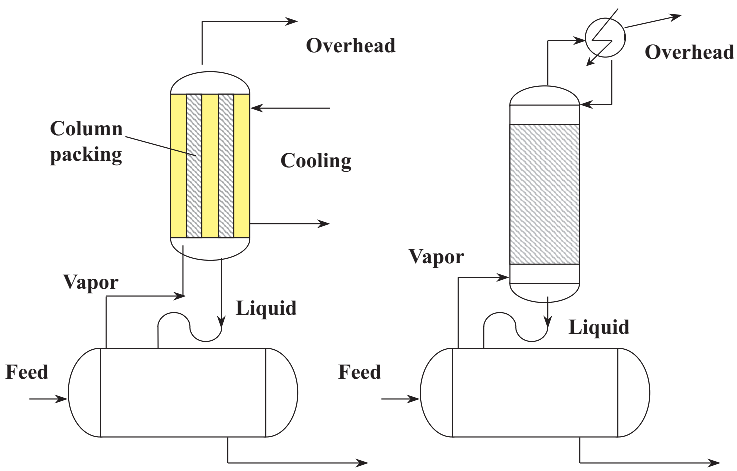


Fig. 5.8. Dephlegmator a non adiabatic rectifier versus a conventional rectifier.

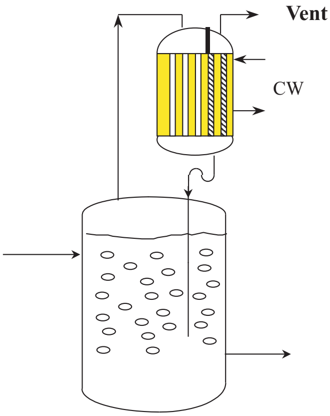


Fig. 5.9. Reactor with reflux condenser and dephlegmator for inert removal.

given separation, while the sub-cooling of the returning condensate is minimal. The combination of functions in this apparatus means that rectification, cooling and the use of a reflux pump might be avoided. The *disadvantage* is that the separation is mostly limited to only three theoretical stages, with application of a rectifying column this limitation is avoided.

The application of side draws, divided wall columns and dephlegmators can lead to large savings in costs. The evolution of a distillation train which has taken advantage of divided wall columns and dephlegmator techniques is shown in Figures 4.16–4.20 in **Chapter 4**, which illustrate the replacement of five distillation columns by two divided wall columns and a dephlegmator. The options for distillation of one to three purified streams in one unit is summarized in Table 5.2. (For ranking of distillation separations with increasing complexity up to four streams, see Table 5.9.)

Table 5.2. Distillation for one, two and three purified streams in one-column configuration.

Distillation	*No. of purified streams*
Flash	0
Stripper	1
Absorber	1
Dephlegmator	1
Simple distillation	2
Distillation with side draw	2 pure, 1 impure
Distillation with purified side draw, (side stripper or dephlegmator/rectifier)	3
Divided wall column	3
Direct coupled distillation	3

5.3.2.4 Direct coupled distillation separations

The divided wall column is an example of a fully thermally coupled distillation. This might also be realized in other configurations. As example, we consider an extractive distillation column (Figure 5.10). In the top section of the column there is a specification on heavies and solvent, and the conventional concept used two columns for these separation. Another coupling for an extractive distillation column is a combination with the solvent stripper is pictured in Figure 5.11, (Emmrich et al. 2000. of

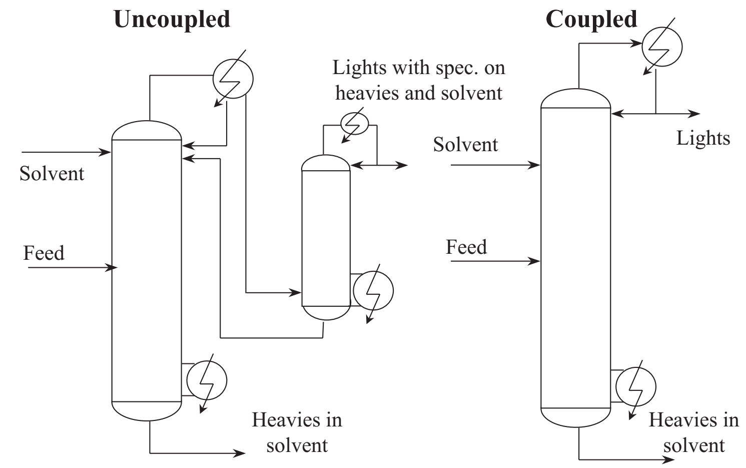


Fig. 5.10. An extractive distillation with two specifications at the top product, heavies and solvent, uncoupled and coupled.

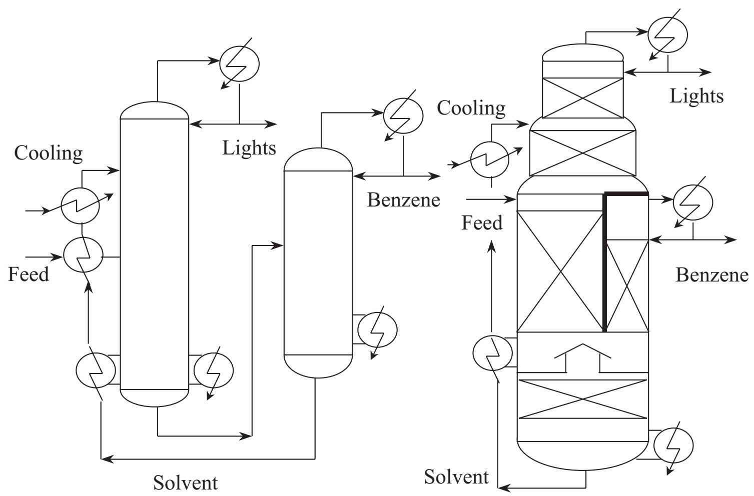


Fig. 5.11. Conventional two columns versus a thermally coupled extractive distillation (Emmrich et al., permission of Kruppe Uhde).

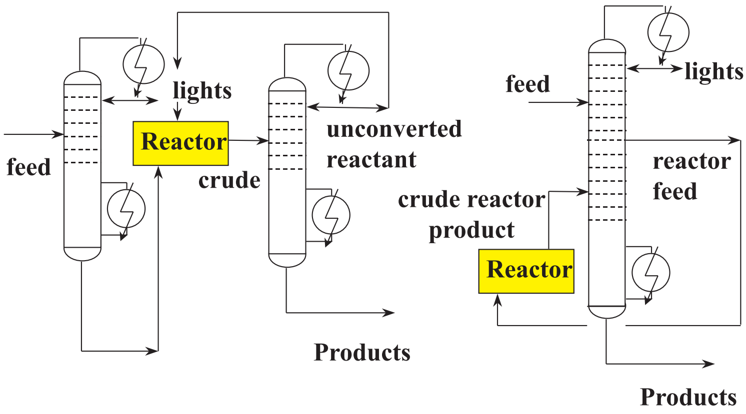


Fig. 5.12. Two separate columns versus one thermally coupled column.

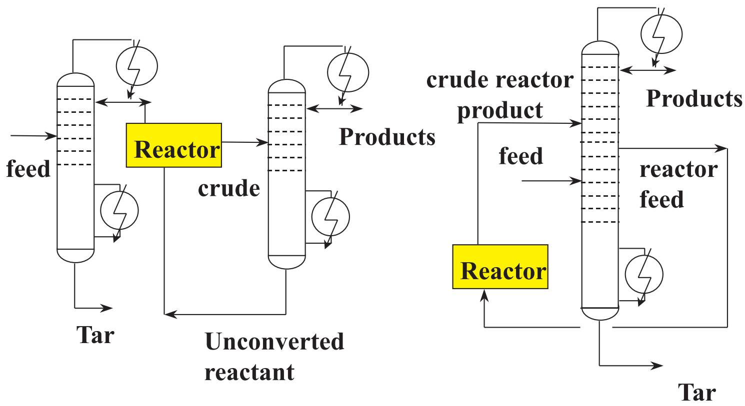


Fig. 5.13. Two separate columns versus one thermally coupled column.

Krupp Uhde). In this industrial example three columns are replaced by one column. The thermal coupling of two distillation columns is also shown in Figures 5.12 and 13. Here, two columns – one in front of a reactor and one after the reactor – are combined in one column. New concepts apply to coupled distillation separations, if the situation permits. For more details, see Section 5.6.1.5.

5.3.3
Extraction, Evaporation, Extrusion

Conventional extraction was carried out in mixing vessels, followed by a gravity separator (Figure 5.14). Due to this rather complex configuration the number of stages were minimized. One improvement to be realized was to replace the mixing vessels with static mixers, although pumps were also used as mixers. Another improvement realized was to integrate the mixing vessel in the separator (Figure 5.15), and the introduction of an extraction column to realize more extraction stages and thus higher extraction efficiencies. These improvements are currently included in the application of several extractions in one column (Figure 5.16), an example of coupled functions. The reduction of equipment of the wash section (see Figure 5.14) to the integrated wash column of Figure 5.16 was that six vessels were replaced by one column, while a total of two pumps (plus their installed spares) could be removed, assuming that the feed pumps would be needed in both situations

The functions avoided are intensive mixing and pumping, while extraction functions are combined with higher extraction efficiencies due to more stages being installed. The elements behind the avoidance can be analyzed. It is noted that the "do-undo-redo" activities (or, in this example, mixing-settling-mixing) were the opportunities for elimination. The design improvements realized were less capital and greater extraction efficiencies, the last point resulting in less solvent circulation with smaller purification equipment. Although the techniques described above are not new, it is their implementation which is still lacking behind, and which deserves to be considered under "simplification".

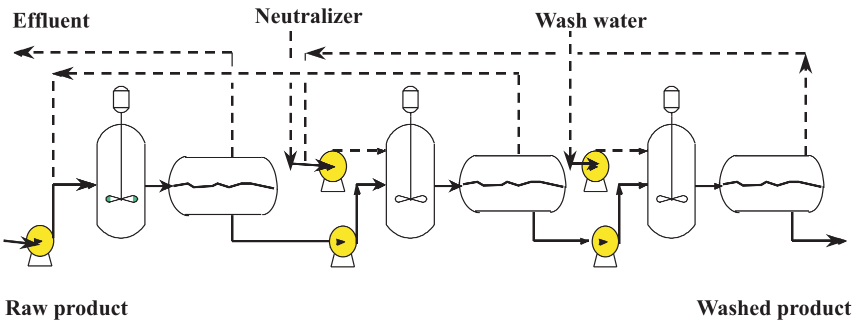


Fig. 5.14. Two sequential extraction wash steps consisting out of respectively two and one stage(s).

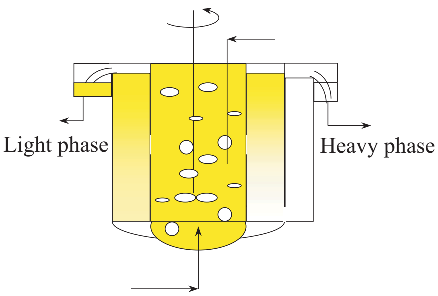


Fig. 5.15. Mixer settler in one cylindrical containment.

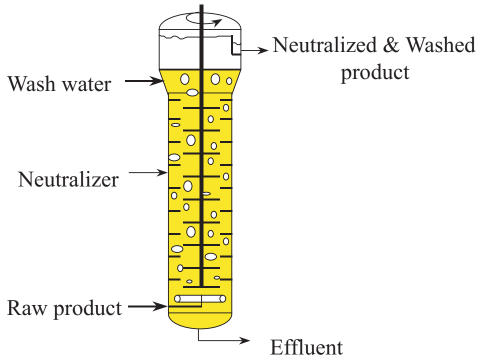


Fig. 5.16. Wash column with two extraction functions and more equilibrium stages.

5.3.3.1 Evaporators

These are used to concentrate a certain process stream by removal of a volatile component. Applications are large energy consumers, and this is the reason why they are often installed in series as multiple effect evaporators. Occasionally, these evaporators are designed as crystallizers (evaporative crystallizers) and are provided with internals to enforce a certain circulation. Such an integrated functionality requires a specific design to achieve the correct balance between crystal nucleation and growth in order to achieve the required particle size, the latter having a major impact on solids removal. An evaporator as a concentrator might also be equipped with a light removal in the top of a rectifier column, while the major vapor stream leaves as a side stream (Figure 5.17).

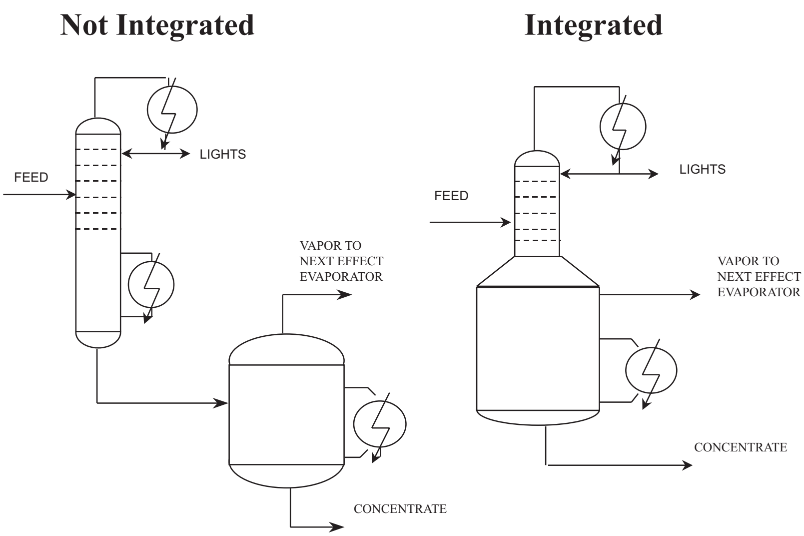


Fig. 5.17. Evaporative concentrator integrated and not integrated with lights removal.

5.3.3.2 Extrusion

Historically, extrusion has always been used for a combination of physical functions. Examples include mixing with other polymers, blending of additives, pumping and product up-grading, as well as the stripping of polymers from volatiles. The stripping technique, through the addition of a stripping agent, has received much attention during recent decades. These techniques were increasingly applied when environmental health requirements for food packaging regarding the removal of monomers and other volatiles became more stringent. More recently, a combination of reaction and extrusion has been applied in this respect (Table 5.3).

Table 5.3. Combination of functions in an extruder.

Extruder	*Application(s)*
Reaction	Co-polymerization
Product upgrading	Heat treatment for product
Blending	Coloring, additives as anti-oxidants
Pumping	Push-through die
Heat exchange	Heating and cooling
Stripping	Removal of volatiles

5.3.4 Furnaces

Furnaces are used for heating purposes, and offer many opportunities for the combination of functions. These are all well known, but are referred to here for completeness.

It is known from energy and exergy analysis that it not enough to achieve high efficiencies based on the net heating value. What is required is not only a high efficiency based on gross heating value, but also a minimum of exergy losses. High efficiencies based on gross heating values can only be achieved by taking advantage of the heat of condensation of the flue-gases, as is practiced in some gas-fired furnaces. Minimum exergy losses are achieved by exchange of heat with a small temperature differences between flue-gases and other streams; this is realized by stepwise heat exchange. As mentioned above, it is clear that the design requires careful optimization of the energy household of a furnace, see Figures 4.39 and 4.40. The standard functionality for combustion equipment is:

- power generation by gas turbine;
- reaction heating
- high-temperature process heating;
- medium-temperature process heating; and
- low-temperature process heating.

In case a gas turbine is not foreseen, the cascade cooling follows the following steps: (i) high-temperature process heating; (ii) medium-temperature process heating; and (iii) air and fuel preheating.

In the above process, heating might include steam generation to achieve a correct energy balance. One design for a furnace for high-temperature reactions is that of a calcination reactor (Figure 5.18). The furnace, which is of a staged, fluidized bed

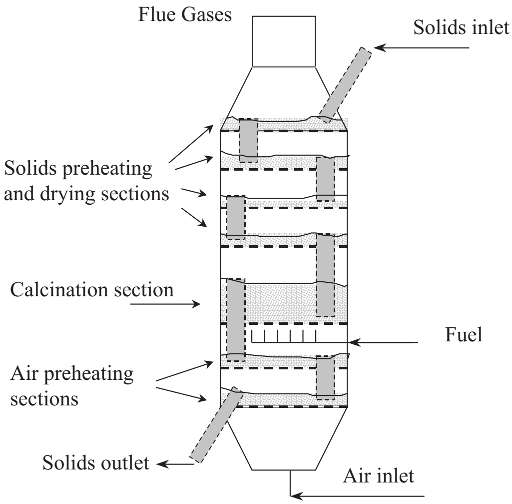


Fig. 5.18. Calcination furnace: multi-stage fluidized beds.

concept, starts at the cold air side with air preheating stages, and this is followed by calcination with fuel as energy source, together with several preheating zones where the feed material is preheated and dried. Clearly, this design is an example of integrated functionality. An overview of the different functions in a furnace are shown in Table 5.4.

Table 5.4. Combination of functions in a furnace.

Furnace	*Application(s)*
Reaction	Steam cracker, syngas production
High process temperature > 250 °C	Process superheater, steam superheater
Medium process temperature, Medium pressure steam	Process heater, evaporator
Low process temperature < 150 °C, Low temperature steam	Process heater, condensate heater
Air/fuel preheating	Flue gas cooling
Gas turbine	Power generation

5.4
Integration of Process Equipment

In this section, we will concentrate on the integration of equipment. The difference between integration and the combination of process function is explained by the heat recovery in the following example. The integration of a vent condenser with another condenser represents integration of equipment, but modification of the vent condenser to a dephlegmator (where rectification and cooling are combined) is a combination of functionality (see Figure 5.9). Some examples of integration of equipment are described below, though the list is far from complete, there being many opportunities within the different processes.

Reactors often have integrated equipment, such as:

- Internal cyclones in fluidized bed reactors.
- Jacket or coils in kettle reactors
- Reflux condensers on top of kettle reactors; this solution is cheaper than recycle cooling (Figure 5.19).
- Integration of adiabatic beds, such as radial reactors, in one shell, and occasionally integrated with an inter-stage exchanger (an example is an NH_3 reactor).
- Integration of horizontal adiabatic beds with inter-stage tubular reactor (Figure 5.20). This example shows a flue-gas-heated system for a styrene reactor (other systems exist with molten salt heating, for a similar application). Exergy-wise, the molten salt system is more efficient as the molten salt can be recycled at a higher temperature level, and this resulted in less generation. (Pumping can be carried out higher temperature compared with compression of gases).
- Integration of three isothermal CSTRs in series by an adiabatic CSTR, and an adiabatic plug flow reactor all in one vessel (Figures 4.7). This was achieved by lowering the feed inlet temperature and slightly increasing one of a reactant flow.

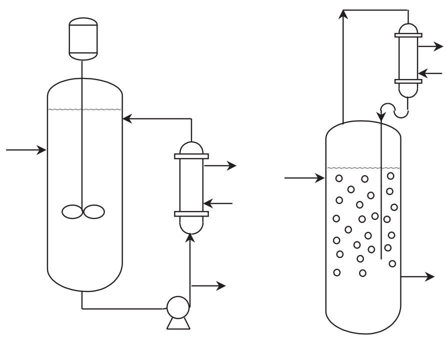


Fig. 5.19. Reactor with recycle loop versus a reflux condenser.

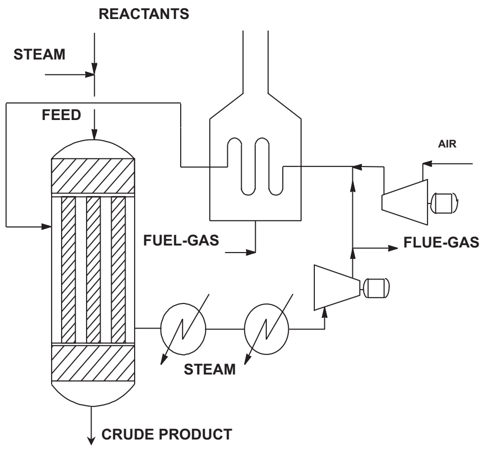


Fig. 5.20. Adiabatic bed–Heated case tubular part–Adiabatic bed of a low capacity styrene monomer process with flue gas heating.

Distillation always offers the opportunity to integrate adjacent equipment with or around distillation columns (Meili, 1997):

- Reboilers for small columns; this often done using a vertical shell and tube exchanger in the bottom of the column. For larger columns, a horizontal tube bundle is installed in the bottom, making cleaning relatively easy.
- Overhead condenser on top of the tower with reflux collection in the top tray (Figure 5.21). This concept is also applicable for air-coolers which are placed vertically in a triangular configuration at the top of a column.
- Compact heat exchangers; manufacturers such as Alfa Laval promote installation of these exchangers for reboilers and overhead condensers.
- Overhead condenser integrated with vent condenser and reflux drum (Figure 5.22).
- Knock-out drum in the skirt of the tower.
- Columns on top of each other are seldom applied, and only when the available area is quite restricted. This should not be confused with coupled distillation columns (see Figure 5.11) and another configuration (see Figure 5.12).
- Demister in the top of the column to avoid carry-over of liquid in high-velocity applications.
- Settlers in reflux drums, particular applied to the separation of heterogeneous azeotropes.

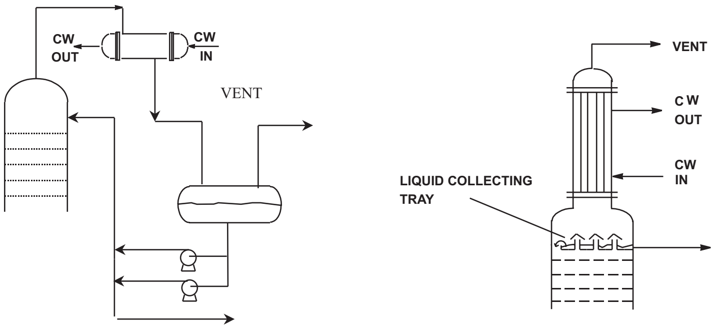


Fig. 5.21. Overhead system with reflux condenser, drum and pumps versus an integrated design.

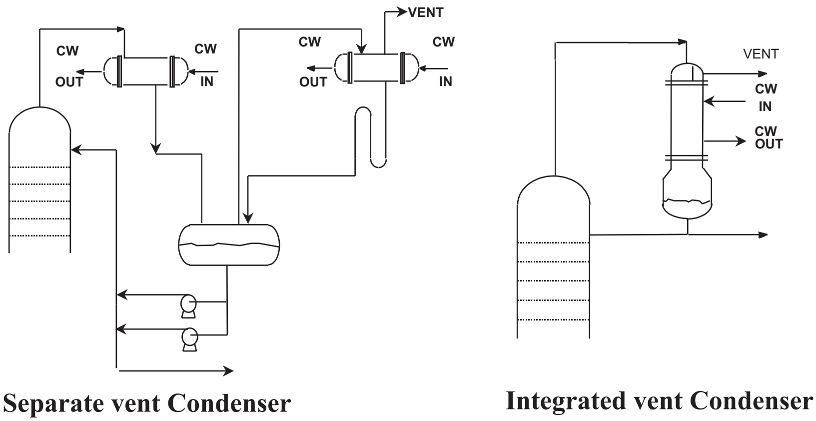


Fig. 5.22. Integration of vent condenser and reflux drum within the overall condenser.

Other applications include the following:

- Demister in knock-out drums and liquid phase separation in the same vessel (three-phase separator).
- Coalescer and settler in one vessel.
- De-aerator stripper on top of a boiler feed water drum.
- Combinations of heat exchanger in one support, as for air coolers, where more coolers are installed in a bank.
- Multiple heat exchangers in one compact system.
- Settler included in the extraction tower.
- Mixer settler in one vessel (see Figure 5.15).
- Flare drum incorporated in the stack (Figure 5.23).

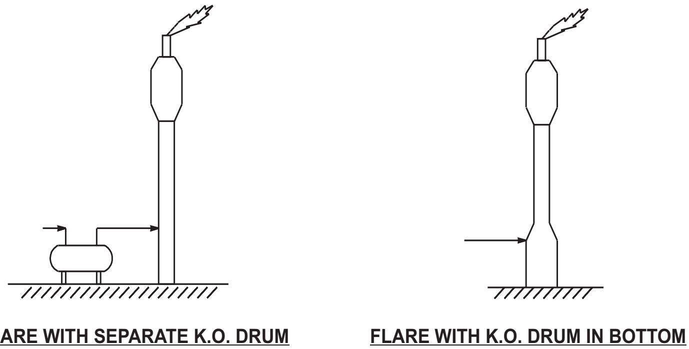


Fig. 5.23. Integrated flare and knock out drum.

5.5 Intensification of Process Functions

During the 1970s, a number of initiatives were taken at ICI to make considerable reductions in the cost of process plants (1^{st}, 2^{nd}, 3^{rd} Int Conf on Process Intensification) The approach taken was to reduce the size of the equipment to a large extent; this, next to cheaper equipment, would result in much lower installation cost. Radical approaches were stimulated to achieve the required scale reductions through intensification. Although the objected scale reductions have, at the beginning of the twenty-first century, been realized only to a limited extent, these objectives are still in place within academic circles. It is clear, however, that new developments take considerable development time and much persuasion before being applied at industrial scale. One area which received particular attention was the reduction of distillation equipment, these generally being the largest-sized equipment in chemical plants. The approach taken was to exploit the advantage of centrifugal fields to enhance separation and transfer (Ramshaw, 1987, 1995). The reduction in the size of distillation columns through this technique has not been realized at industrial scale. Nevertheless, the emphasis on process intensification has resulted in much success and remains a drive for research. The major developments will be discussed below, although the discussion is limited to areas that are currently applied (or are at the point of being applied) at industrial scale.

Process innovation commences from a background of:

- Stirred tank reactors have bad mixing characteristics for heterogeneous systems, as well as small heat and mass transfer coefficients that often limit the performance.
- Bubble and packed columns for heterogeneous reactor systems are often mass- or heat transfer-limited. (For reaction systems that are limited by mass and heat transfer, large improvements can be expected by intensification of the rate-limiting steps.)

- Distillation equipment requires low velocities, to achieve a gravity separation between vapor and liquid and this results in large diameters; relatively low velocities do not enhance mass transfer.
- Shell and tube heat exchangers have a relative low surface area per volume.

While these background points were seen as starting points for process intensification, the efforts taken can be divided into the following categories:

- Building more compactly: mass and heat transfer exchangers increase the effective surface area per unit volume M^2/M^3.
- Increase heat, mass, and impulse transfer.
- Benefit from centrifugal forces ("Higee").
- Overall process improvements (see Section 5.6).

These categories have been selected to emphasize the technique of process intensification, rather than focus on the unit's operation and its applications.

5.5.1
Building More Compact Units

The concept here is to create more separation area per unit volume. The developments in this field were not among the first to be evaluated, but were an intensified continuation of ongoing developments.

5.5.1.1 Phase separation

The technology for phase separation provided more separation area in gravity separators by the installation of tilted plates in the separator, thus reducing the vertical distance that the particles/droplets must pass before separation (Figure 5.24). These improvements were greatly appreciated by the offshore oil industry to reduce the oily water separator sizes. The onshore industry also improved the performance of these separators by increasing the separation area within the existing units. The same principle was applied in centrifuges, where tilting plates were introduced to shorten the separation distance and so increase the separation capacity of the unit.

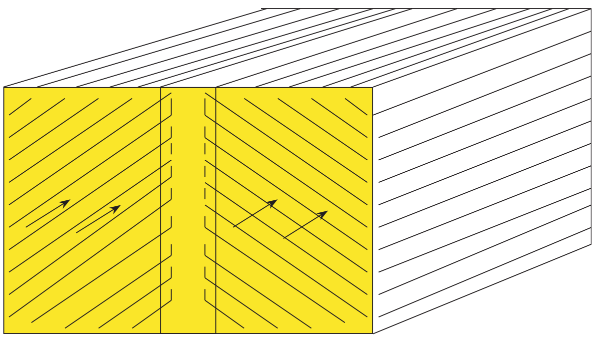


Fig. 5.24. Tilted plate separator.

5.5.1.2 Heat transfer

During the 1970s, heat transfer was somewhat limited to plate frame heat exchangers with a larger surface-to-volume ratio than shell and tube exchangers. These units found wide application in the food industry to treat sticking and fouling streams, but were used to only a limited extent in the chemical industry. Their major drawback was that they were fitted with numerous large gaskets that had a tendency to leak. The improvements expected during intensification (this was also driven by the motor car industry, which had a need for reliable tight, low weight, compact heat exchangers), were large area/volume, tight systems, multi-stream units, and suitable for multi-phase applications. The leading vendors in this field accepted the challenge, and initially the system was tightened by the use of semi- or total brazing or welding techniques to limit/eliminate the need for gaskets. The next step was to increase the surface area by introducing fin plate heat exchangers, or even micro channel heat exchangers, to increase performance. This brought compact exchangers of 1000 M^2/M^3. The construction options of the device made application as evaporators and condensers and also multi-stream designs a reality. Enhancement of the heat transfer coefficient was realized by the application corrugated plates. The drawback of the exchangers is that applications are restricted to nonfouling systems. The advantage, next to the size and low cost, is the performance which makes designs with a small temperature approaches attractive. Thus, higher energy utilization is to be effected, which is inclusively realized by the countercurrent operation. For one-phase systems this can conventionally be realized by multiple shell and tube exchangers in series, though at very high cost (Thonon and Mercier, 1997; Edge et al., 1997). The applications of compact heat exchangers are quite extensive in the automotive industry, and in air-conditioning, refrigeration and liquefied gas applications. Further applications at the process industry are at hand, but "trend-setting" applications such as reboilers and condensers are needed to advance this situation. Further application in this area will push the shell and tube heat exchangers into the role of museum pieces.

Future developments might lead to applications such as reactive heat exchanger for highly exothermic, rapid reactions, including those of catalytic plate reactors, and developments are ongoing in this area.

5.5.1.3 Mass transfer

Mass transfer operations of gas–liquid systems urgently require size reduction. Efforts in this direction, based on the use of centrifugal fields to enhance phase separation and mass transfer, have not been practicable on an industrial scale. Mass separation by membranes offers another approach to reduce the size, and surface-to-volume ratios over 1000 M^2/M^3 have been exceeded by far the ratios of conventional, direct contact gas liquid separators (typically 100 M^2/M^3) (Jansen et al., 1995). Gas absorption might be physical or reactive, and no differentiation will be made between these. Membrane separations such as reverse osmosis, ultrafiltration and microfiltration are now considered to be standard technology. For the operation of membrane gas absorbers, the majority of conventional absorbents can be used, although it is vital that the absorption liquid does not penetrate the membrane. For nonwetted, microporous membranes it has been shown that the resistance due to the membrane is low, or even insignificant. For wetted membranes, the resistance of the membrane severely affects the absorption rate. Wetting is influenced by the pore size, pressure difference across the membrane, and the interaction of the absorption liquid with the membrane material. This phenomenon is described by the Laplace equation:

$$\Delta P = -2\ (\gamma/r)\cos\Theta, \tag{1}$$

where ΔP is pressure difference (N/m^2), γ is surface tension liquid (N/m), r is pore radius (μm), and Θ is the contact angle.

The membrane will not be wetted if the contact angle is >90° and the pressure difference is limited for a certain pore size. Membrane absorbers can be operated at relative very low liquid flow rates which are not achievable by conventional absorbers such as gas/liquid mass flow ratios of 1000. The low liquid loads has an impact on the regeneration unit, which also can be smaller in size

The absorption liquid might contain salts of amino acids or promoted amino acid solutions for CO_2 removal. Applications tested at the industrial scale include the removal of CO_2, H_2S and SO_2. A ten-fold reduction in absorber size appears to be realistic.

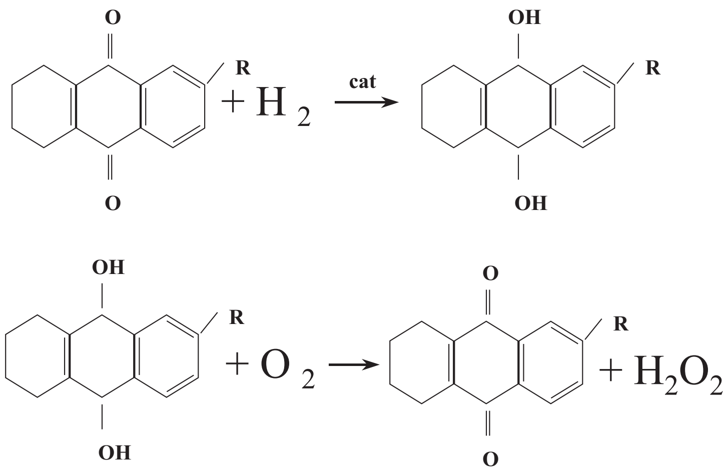
5.5.2 Increased Heat, Mass and Impulse Transport

More than just progress has been made to improve the design of heterogeneous reactors such as stirred tank reactors (STRs), bubble columns, and trickle flow reactors. Indeed, the challenge is to improve the rate-limiting step as heat or mass transfer, and this forms the basis for reductions in equipment size. The improvements made in this respect may be called "spectacular", and some examples (with industrial applications) are mentioned briefly here. The improvements made will depend on the ratio between transfer rate and reaction rate, starting from the historical situation.

Originally, the *nitration of aromatics* was a mass transfer limited operation between two liquid phases – the aromatics and the acid stream (HNO_3 in H_2SO_4) (Hauptmann et al., 1995). The reaction is strongly exothermal, with the aromatic as the dispersed phase. The reaction was executed in a series of isothermal CSTRs. The HNO_3 is almost fully converted, while the H_2SO_4 is recycled after removal of the reaction water by flashing. To achieve high mass transfer rates in liquid/liquid reaction systems, it is essential that the liquid phases are dispersed, and re-dispersed. This leads to the creation of a fresh interfacial surface that takes part in the high heat and mass transfer rates. The design of a mixing system which accommodates the dispersion and re-dispersion is crucial for performance.

Different technology suppliers have different solutions, but the final result is that a series of CSTRs (three to five, with low performance mass transfer) were replaced by a tubular reactor. The CSTRs design was executed under isothermal conditions, as the "hold-up" of these systems was considerable and could easily lead to a "runaway" reaction. This was the dominant reason why the process was performed under isothermal conditions, with the reaction heat being lost into the cooling water (see Figure 4.8 in **Chapter 4**). The tubular reaction was adiabatic, and the heat could be utilized for downstream separation. This resulted not only in a considerable reduction in reactor cost but also a reduced energy cost. The safety of the process was improved as the hold-up on reacting components was reduced over ten-fold.

Intensification of the *anthraquinone* process for the production of hydrogen peroxide was studied at Kemira (Turunen, 1997; Turunen et al., 1999). The process has an overall process flow diagram as shown in Figure 5.25, with the following reaction scheme:



The oxidation reactor was, in the conventional technology, a packed bed or bubble column for the gas/liquid reaction, with air as the oxygen source. The idea was to intensify this reaction by the replacement of air by oxygen, and intensification of the mass transfer. A tubular reactor provided with mixing elements resulted in high transfer rates (Figure 5.26). The reaction is slightly exothermic, but the high mass flow of the working fluid and cooling did not result in a limitation on heat transfer. The limitation was the flow regime in the tube, where liquid was preferred to be in the continuous phase in order to accommodate high mass transfer rates. This problem was solved by the application of more injection points for the oxygen. The final result was that the reactor volume was reduced by a factor of 10, while the amount of working fluid was minimized and the selectivity increased as less epoxide was formed.

Hydrogenation reactors are subject to intensification, which are gas-liquid-solid systems. The different types of conventional reactors are:

- Slurry reactors as CSTR or bubble columns, where the catalyst is dispersed as very small particles and requires an intensive and expensive recovery system (the catalyst is mainly Pd on carbon, and is of very high value).

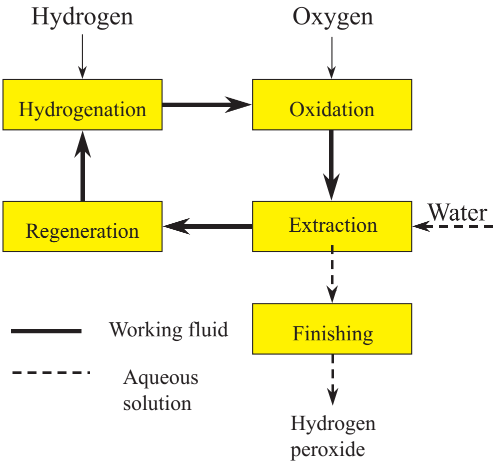


Fig. 5.25. Production of hydrogen peroxide by anthraquinone process (Ref. Turunen, with permission of BHR publ.).

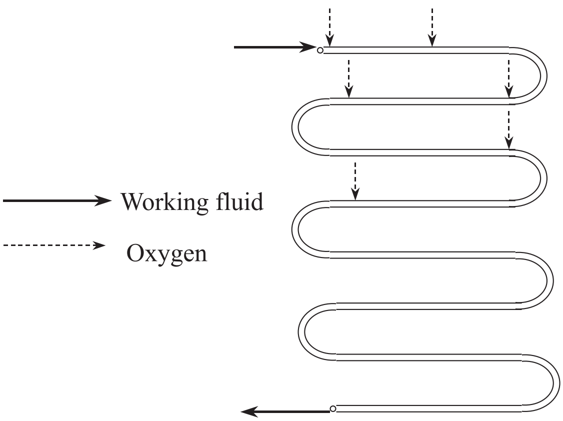


Fig. 5.26. Tubular reactor for oxidation (Ref. Turunen, with permission of BHR publ.).

- Packed columns are another option used when the catalyst is in pellet form, and gas and liquid flow are either co-current or counter-currently operated.

The hydrogenation reactions are both rapid and strongly exothermic, and are limited by mass transfer in conventional reactors.

Different options were experienced to intensify the reactors, although it should be realized that a very wide range of hydrogenation applications exist, from the selective hydrogenation of acetylenes in hydrocarbon streams to the total hydrogenation of nitro-aromatic compounds and many others. Here, the discussion is limited to three-phase systems, where the solid phase is the catalyst. However, it should also be realized that during hydrogenation heat must be removed, as this can also-dominate the design, specifically during total hydrogenation. The options for heat removal are:

- Adiabatic reactor, where the temperature increase of the reaction medium is controlled with recycle of (preferably) the liquid phase due to is higher specific heat and density. This is commonly applied in packed bed reactors.
- Boiling reactor applied with slurry reactors for CSTR and bubble column designs.
- Tubular reactor.

The above ranking order should be seen in perspective of the discussion on the ranking order of reactor design in Section 5.7.1.

The intensification from a mass transfer perspective has been studied by Marwan et al. (1997) in co-current, down-flow contact reactors (gas dispersed in liquid) for different reaction systems. This contact system can be applied for slurry as well as packed bed reactors, although a packed bed reactor will often be favorable to avoid the need and cost of catalyst recovery. The principle is that the gas is co-currently with the liquid dispersed by high-velocity jet in down flow, while the liquid is the continuous phase. The high degree of shear and turbulence created results in good gas-liquid contact and high interfacial area, resulting in high mass transfer rates. The dispersion in the column extends down the column, where coalescence of bubbles occurs; these rise back up the column and re-disperse higher up. This concepts leads to much smaller reactor compared with CSTRs, and also higher selectivity, depending on the reaction mechanism.

Another solution was reported by Turunen (1997). A packed bed reactor was developed with the catalyst fixed in pockets inside a structure made of metal gauze. Gas liquid is moving co-currently in the open channels, and gas is dissolved in the liquid. The liquid penetrates through the gauze into the catalyst pockets, where reaction takes place. The disadvantages of catalyst recovery in a slurry reactor may be overcome by this solution.

The application of co-current, down-flow gas liquid reactor through packed beds (trickle beds) with self-generating pulsing flow is a technique to enhance mass transfer (Tsochatzidis and Karabelas, 1995). The advantages are the intensive interaction between the phases, resulting in high heat and mass transfer rates through renewal of interfacial areas, reduced back mixing, and elimination of hot spots. However, this has as a disadvantage that relative high flow rates are required to achieve pulsing flow with short contact times. The application is therefore limited to fast chemical reactions.

Induced pulsing flow was also studied by Tsochatzidis et al. (1997). These studies emphasized the introduction of induced pulses with the liquid stream at a relative high frequency. The results indicated an enhancement of mass transfer in an operable area where self-generating pulsing flow was not applicable. The technique appears promising, but needs further investigation.

Induced pulsing flow has also been applied for some time in extraction columns, either by the introduction of pulsations with the feed pumps or with an external pulsation device. Alternative designs applied here are the introduction of a rotating disc or vertical displacement of discs which are assembled on an axis. These all have the purpose of intensifying the mass transfer.

Currently, a supersonic, two-phase flow mixer is under development at Praxair (Cheng, 1997). The concept is based on the creation of very small droplets in a gas stream, through a supersonic, two-phase mixer The application area would be very rapid gas-liquid reactions.

5.5.3
Benefits from Centrifugal Fields: "Higee"

Centrifugal fields have, for many years, been successfully exploited in phase separations. The application of cyclones in gas/solid, gas/liquid separations are well known, their limitations being mainly due to particle size and scale-up (larger-scale cyclones have a lower separation efficiency). Hydro-cyclones, which have found application in liquid/solid separations, are very simple, robust devices and have a wide field of application. Likewise, centrifugal devices are widely used for liquid/solid and liquid/liquid separations. The application of multi-stage centrifuges for liquid/liquid extraction is also an intense operation which is often applied where there are only small differences in the density of the materials to be separated. This technique is of particular interest in the pharmaceutical industry, where advantage is taken of the small hold-up. Although during the past few decades several types of centrifugal separation apparatus have been developed by the manufacturers, it was only during the 1970s that process intensification initiatives were started, driven mainly by ICI.

The idea was to reduce the size of equipment considerably in order to achieve much lower capital costs (Ramshaw, 1987, 1995). It was concluded that the size of equipment was often determined by phase separation, which in turn restricted the speed at which transfer processes could be carried out. By applying a centrifugal force, phase separation could be improved to provide higher processing speeds, and this in turn should result in improved mass transfer. In terms of a gas/liquid column, the diameter should be decreased (higher velocity), but the height must also be reduced by improved mass transfer and phase separation. The initial industrial results for acceleration-induced gas/liquid separations were limited, and developments into the use of centrifugal forces over a wide range of operations continued in research, especially as the potential benefits were realized and were not under debate. Some details of these ongoing research efforts are summarized below.

Centrifugal forces have been applied for de-sorption, for example of de-aerators of water streams. In the case of oil field flooding water, de-aeration vacuum towers were installed. The first development of a so-called high-gravity ("Higrav") machine was at the university of Beijing, and this resulted in a range of plant-scale machines that were tested successfully in the field (Zheng et al., 1997). The technique is also applicable for de-aeration of boiler feed water.

A *rotating machine* was developed as the heart of an absorption heat pump by Ramshaw and Winnington (1997) at ICI, and-later at the University of Newcastle and at Interotex Lim. The development focuses on a double-effect absorption heat pump and is intended for use in small-scale air-conditioning and refrigeration plants. Field tests of this equipment are currently under way.

Rotational particle separators for dust and mist streams of particle sizes >0.1 μm have been described by Brouwers (1996). The core component of the rotational particle separator is the filter element, which consists of a multitude of small axial channels rotating around a common rotational axis. The gas streams flow axially through these channels, where the particles are centrifuged against the wall. The gases leave the channels, while the particles are collected at the walls where they are periodically removed at high velocities.

Reactive stripping in a rotating packed bed has been used in the production of hypochlorous acid at Dow Chemical (Trent et al., 1999). This problem was recognized as an opportunity to utilize centrifugal techniques by virtue that although the reaction employed:

$$NaOH + Cl_2 \rightarrow HOCl + NaCl$$

had rapid kinetics, the HOCl produced was subject to undesirable decomposition to chlorate. The key to the development of the process was the rapid transfer through the maximum decomposition pH zone, which maximized stripping of the HOCl to the vapor phase. The solution to the problem was found in a rotating packed bed which moved liquid through a porous packing while the gas moved countercurrently. This resulted in an industrial application with the design principle of a rotating packed bed that could be applied to different separations, including gas/liquid or gas/liquid/solid, absorption, and adsorption (Figure 5.27).

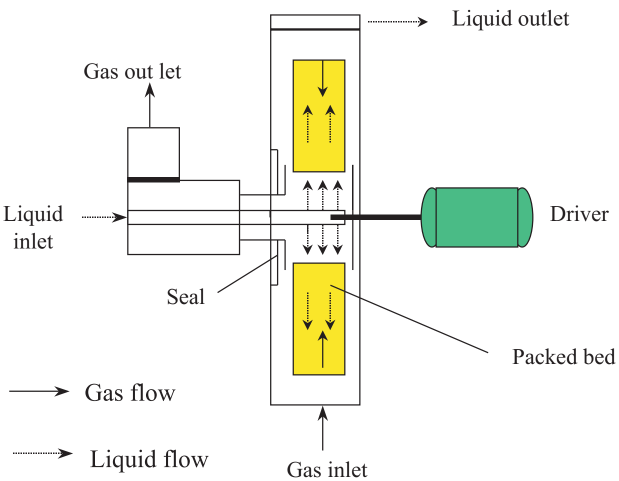


Fig. 5.27. Rotating Packed bed applicable for fast; G/L and F/L/S reactions, absorption, adsorption.

Polymer devolatilization and pelletization have also been developed within a rotating packed bed, mainly as the result of increasing requirements for low residual monomer levels within polymers. The technology (Cummings et al., 1999) is a combination of a rotating packed bed and a centrifugal pelletizer, and was developed to enhance mass transfer in order to improve polymer devolatilization. Combining the two unit operations led to the creation of a device that was significantly smaller and cheaper than existing solutions, and field testing of this unit is currently in progress.

A summary of process intensification is provided in Table 5.5.

Table 5.5. Summary of process intensification.

Process intensification	*Application*
Build compact	
Tilted plate separators	Gravity and centrifugal separations
Heat exchangers	Air separation
Mass exchangers	Membranes for reverse osmoses, ultra-filtration, membrane absorbers
Increase heat/mass/impulse Transport	
Static/vortex mixers	Fluid mixing G, L, G/L, L/L
Pulse flow, self generating/induced	Trickle flow reactors, extraction
Supersonic mixing	
Centrifugal field	
Cyclones	G/S, L/S, L/L
Centrifuges/decanting centrifuges	L/S, L/L
Rotating packed beds	Reaction
Rotating packed bed	Devolatilization
Rotational separators	G/S, G,L particles/droplets <0.1 μm
Rotational de-sorber/de-aerator	G/L
Rotating machine	Absorption heat pump

5.6 Overall Process Simplification

Overall process simplification relates to a higher design level than has been described above, and is based on the simplification and intensification of single units, or the combination of functions such as reactive separation. The application of overall process simplification is based on a review of the overall process for improvements, and may be subdivided as:

1. Overall process design improvements
2. Single train design, scale-up of systems
3. Strategy around supplies and storage
4. Strategy around single component design

5.6.1
Overall Process Design Improvements

In order to achieve simplification of the overall process, a careful examination must be made of the overall process design improvements. These simplifications may be found not only in the overall process flow diagram, but also in the finer details which might, in fact, have a greater impact. The techniques mentioned in the previous sections which have been directed at specific units clearly contribute to an improved design. However, they also need to be judged from an overall process perspective, and therefore they will be referred to here in a wider context.

Process synthesis requires the efficient selection, sequencing, and integration of the different reaction and separation units, as was described in **Chapter 4.** This is a very difficult task, as can be concluded from the options for simplification described in this chapter. It is important to understand that the alternatives shown represent only the "tip of the iceberg". Here, an improvement in a steam system serves as an illustration of how simplification can still be effective in a highly conventional process. A conventional system (Figure 5.28) has a de-aerator and a slightly over-pressured steam drum/tank which supplies the steam for de-aeration, followed by chemical dosing to remove remaining oxygen. The system loses some water through the vent, as well as an amount for process steam injection and condensate usage. This flowsheet represents an accumulation of effects resulting in water usage, energy losses, chemical dosing, and water pretreatment for water losses.

The alternative (Figure 5.29) is based on the prevention of steam or condensate injection for process reasons. A low-pressure condensate flash drum is provided where the flash steam is used by a process consumer. With these modifications, the make-up is absolutely minimized, and so is the introduction of oxygen. As a result, the de-aerator and condensate pump can be removed, and the chemical dosing required is minimal as no oxygen enters the system. The ultimate result is less energy losses, lower capital and operational costs, and minimal water treatment costs. This is a typical overall simple and robust design improvement.

The overall process design might be examined from different perspectives in order to identify opportunities for improvements. Indeed, the following pathways might be explored to improve the overall design:

- Operation at 100% conversion
- Additives and supplies
- Prevention of waste streams
- Adiabatic operation of reactors
- Combination and coupling of functions (see Section 5.3.2 for coupled distillation separations)
- Energy integration.

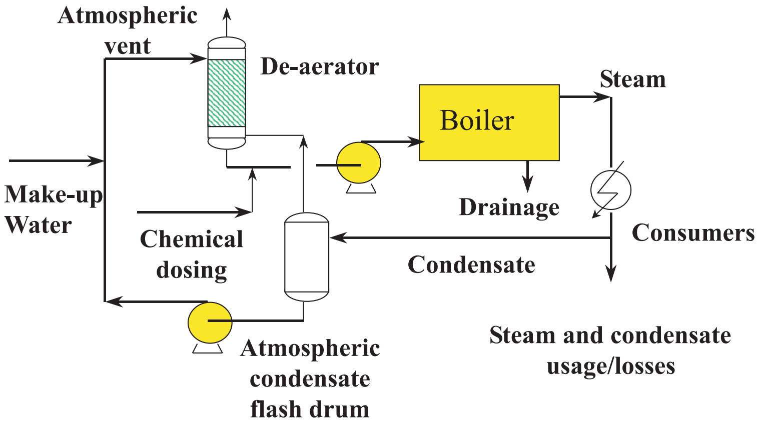


Fig. 5.28. Conventional feed system for steam boiler with considerable make-up to compensate for vent/usage/losses/drain, and energy losses from the atmospheric flash steam.

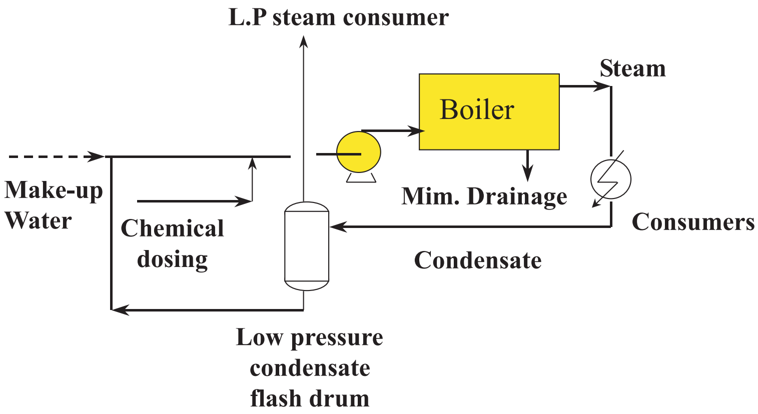


Fig. 5.29. Feed system for steam boiler with hardly any make-up to compensate for losses, no de-aerator and condensate pump nor energy losses.

5.6.1.1 Operation at 100% conversion

This is carried out in order to avoid expensive recycle systems. although it is often not an option for all reactants, and especially not for equilibrium reactions. This last point might be exploited by shifting the equilibrium by reactive distillation or other product removal techniques such as absorption, adsorption, or extraction. An option for nonequilibrium reactions is to design the reactor system for complete conversion of one of the reactants.

5.6.1.2 Additives and supplies

It is possible that minor amount of additives might be used, but with major consequences. A careful review of all process additions and their impact might provide surprising results. Let us consider the inhibitor and its solvent used as an additive for polymer prevention. Current designs apply extensive recycling in order to reduce environmental losses. Questions about additives include:

- Is it understood what happens to the inhibitor and its solvent during processing?
- Are they degraded during processing?
- Do these components or their degradation products leave the process, and if so, at what point?
- If accumulation occurs, where might this happen, and what will be the consequences?

Several examples exist of additives and their solvents which require process "add-ons" to overcome their effects. It is not uncommon to find a washer or vent-gas scrubber (or even an oxidizer) as an add-on provision. One might consider what type of provisions are required if these chemicals were toxic with regard to biological treatment. For example, the chemicals might contain nitrogen, and this would require an additional step in a waste treatment plant, or it might add to the NO_x load. These provisions might be avoided by using other inhibitors or solvents.

A good choice for the selection of a solvent for additives is a pre-existing process component.

The *type of neutralizing agent* might also be challenged. A neutralizer such as caustic soda might result in the need for an expensive step to remove the sodium salt produced. Replacement with NH_4OH might be beneficial if the ammonium salt formed were to remain in the product, but if it were-to appear in the wastewater, it might lead to a high nitrogen load, or its degradation might impact on the NO_x load. Another option might be to use an organic base that would remain in the product.

A seawater cooling system was badly affected by mussels growing in the tubes of heat exchangers. Periodic chlorine "pulses" to prevent mussel growth were effective, but they introduced a very toxic and dangerous chemical at the chemical complex. Replacement of chlorine by hypochlorite solutions was safer and avoided the need for many on-site provisions to cope with a potential emergency situation (Paping et al., 1999).

Chain transfer agents are quite commonly applied in polymerization processes, and have also been the subject of critical reviews. The removal of these components can lead to a need for expensive recovery systems. One process which was brought to the author's attention used a chlorinated hydrocarbon that required not only an extensive recovery system but also an incinerator with Cl destruction and HCl recovery. Time spent in developing a less harmful transfer agent that was able to remain in the product was successful, and implementation of this scheme resulted in a much simpler overall process.

5.6.1.3 Prevention of waste streams

The prevention of waste streams results in a need for fewer facilities to recover or degrade the waste that otherwise would reach the environment. This is not limited to continuous streams, but includes discontinuous streams and even releases from emergency systems. All such streams need careful evaluation to prevent their formation, before recovery systems are considered. An example is the prevention of emergency relief on ammonia storage described in **Chapter 3** (see Figure 3.6). Here, instrumental protection took over safeguard of the tank from a pressure relief system, though this required a different design strategy. The pressure relief system protects against any overpressure, and is sized according to the largest load, but for the instrumental protection system there is no relief device, which means that the system must prevent any potential over-pressure at a required level of reliability.

A central header system for collection of the emergency relief devices of process systems is something which needs to be re-considered. Such a collection system results in a need for large recovery or destruction units. Another approach is to align relief devices with an internal process vessel, which can largely avoid or minimize any need for external relief. The same approach must be applied for draining systems, as any drain into a central system often makes recovery for process re-use more difficult. The re-routing of drains for internal re-use is worth studying, and in such a case the drains of one particular process section might be collected and recovered in the same section.

5.6.1.4 Adiabatic operation of reactors

The adiabatic operation of reactors has a wider impact than does the reaction section alone. On comparing the three cooled CSTRs with the adiabatic CSTR and plugflow reactor of Figure 4.7 in **Chapter 4**, it is clear that there is a large difference which is not limited to a low cost reaction section. For the overall process, there is an impact on the selectivity, and the conversion energy drops due to usage of the heat of reaction; this results in a smaller steam system, while the role of the cooling water system, together with its make-up water, is reduced. The same applies to the example of the nitration reactor (Figure 4.8 in **Chapter 4**).

The advantages of adiabatic reactor designs therefore have a high priority in the ranking for simple designs (see Section 5.7.1).

5.6.1.5 Direct coupling of separations

Several examples of direct coupled applications were discussed earlier in Section 5.3.2.4, the divided wall column being the most generic application. The example of extractive distillation combined with a rectifier (see Figure 5.11) is achieving wider application.

Searching the process for opportunities in this respect led to a number of applications (see Figure 5.12), but in this case two distillations are direct coupled, thus combining a separation before and after a reactor. This type of application is encountered around a reactor system when the feed contains lights that are to be removed, when the conversion in the reactor does not run to completion, and when the reactor products are heavier than the unconverted feed. A similar concept can be applied when the feed contains heavies to be separated, the conversion is incomplete, and the products formed are lighter than the feed (see Figure 5.13).

A generic rule is that a feed to a reactor system can be distilled coupled with a reactor outlet stream if:

- the reactor conversion is incomplete;
- the boiling points of heavies and light at a selected pressure level can be handled with practical utility conditions;
- the feed (reactant) contains lights and the reactor outlet stream or its purified stream contains heavier products compared with the feed (see Figure 5.12); and
- the feed contains heavier, and the reactor outlet stream or its purified stream contains lighter, products for separation (see Figure 5.13).

The evolution of the separation train as shown in Figures 4.16–4.20 in **Chapter 4** is an ultimate example of the combination of separations.

The coupling of extraction steps is an other opportunity that is practiced specifically in washing sections (see Figure 5.16). The coupling of an absorber and a stripper is practiced in nitric acid plants (Figure 5.30), where the NO_x vapors are absorbed in water under the formation of HNO_3. The nitric acid leaving the absorber contains dissolved NO_x, which must then be removed. By installing a stripper under the absorber, the functions are directly coupled. The above examples represent only a few of the opportunities that engineers have realized, a short summary of which is provided in Table 5.6.

Direct coupling of separations, with the exception of divided wall columns, are difficult to identify in generic rules as they depend very much on the process. The coupling of separations demands creative thinking by the designer – and a need to reconsider their travelling along the “paved roads” of performing tasks in a sequential order.

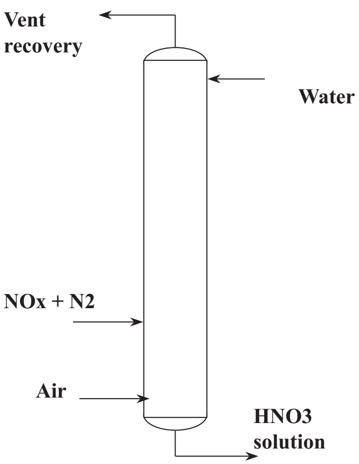


Fig. 5.30. Absorption combined with stripping in an nitric acid plant.

Table 5.6. Some directly coupled separation functions.

Functions	*Applications*
Divided wall column	Figure 5.7 Replacement two distillations
Two direct coupled distillations	Figure 5.12–5.13 Feed and outlet of reactor
Extractive distillation with overhead stripper	Figure 5.10 Benzene from non-aromatics
Extractive distillation with solvent stripper	Figure 5.11 Benzene from non-aromatics
Absorber with stripper	Figure 5.30 HNO_3 absorption and stripping
Several extractions in one column (2 or 3)	Figure 5.16 Neutralization, washing
Stripper with evaporator	Figure 5.17 Evaporative concentrator
Filtration and washing	Filter cake wash L/S
Centrifuging and washing	Filter cake wash L/S
Reaction in furnace with drying and cooling	Figure 5.18 Calcination furnace

5.6.1.6 **Energy integration**

The overall energy integration needs to include pinch and exergy analysis – both of which are powerful tools (see **Chapter 4**). It is not the intention to repeat here all what was said about energy integration, though it is worth recalling the objectives of pinch analysis:

- Minimize the energy target by modifying the process flowsheet .
- Raise the temperature of energy producers (exothermal reactors, condensers), and lower the temperature of energy consumers (endothermal reactors, reboilers), to enable improved integration.
- Develop the heat exchanger network by clever integration and follow the basic implementation rules referred to in **Chapter 4**:
– Apply process integration in the following order of priority: unit; section; process; site (complex).
– Apply heat exchange between flows of similar heat capacity (mass flow × specific heat).
- Design the process energy system with enough flexibility to avoid excess in steam grids that result in the dumping of steam.

In the previous Section 5.6.1.5, which outlined the coupling of separation units, the focus was on the thermal coupling of units. The main challenge for energy integration is to develop project alternatives that will achieve lower energy targets, based on the flowsheet after any coupling has been studied. The lower targets are to be realized by the adaptation of process conditions to enable surface heat exchange. The options available for modification of distillation column energy conditions (Figure 4.33 in **Chapter 4**) as being a major energy consumer are to:

- adapt the operational pressure/minimize pressure drop;
- change the composition(s) of separation;
- consider using a side re-boiler/condenser;

- consider a vent condenser to increase condenser temperature;
- consider using a direct heat pump between top and bottom;
- use high-flux tubes;
- consider the number of trays or height of packing;
- consider feed preheating; and
- to use a multi (two- to three-) stage distillation.

For a sequence of distillation columns (Figure 5.31), the potential energy saving options are:

- Alternative sequence.
- Three-component distillation, thermally coupled.
- Energy integration (top on bottom or side).
- Partial condenser with vapor feed to next column.
- Side reboilers/condensers.

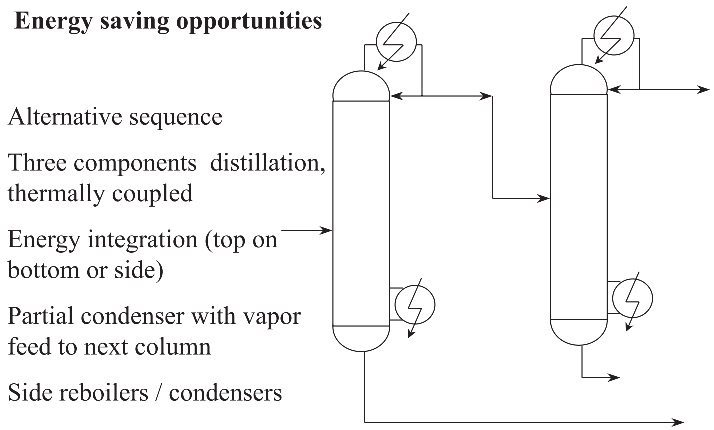


Fig. 5.31. Opportunities to realize energy savings for two sequential distillation columns.

Special attention is required for those temperatures which are higher than the condensation temperature of the high-pressure steam grid.

An exergy-efficient supply of energy at this level is not always easy to obtain. These temperature levels for process heating can be generated in furnaces, but the furnaces have to be provided with a power generator or another high-temperature process demand to achieve a reasonable exergy efficiency. Therefore, opportunities of avoiding these temperature levels must be explored first. The potential energy improvement of a fired re-boiler (Figures 4.36 and 37 in **Chapter 4**) include:

- lower pressure operation;
- allow more lights in the bottom;
- install side reboiler with electric heater in the bottom;

- install side reboiler with superheated steam reboiler in the bottom;
- install gas turbine in front of fired reboiler furnace; and
- install air pre-heater and combine its thermal load with other high temperature process demands.

Other applications will require equally careful study. The need of a furnace is not always avoidable, but it is worth exploring the options. For example, it may be beneficial to know about the initiation of an exothermal reaction say 300 °C (see Fig 4.38). By taking advantage of the superheat in steam, it may be possible to start-up such a reactor; after the reactor starts the reactor system can be self supporting and a furnace can be avoided.

Another known possibility for energy reduction is the application of a partial condenser on a distillation column. In the original flowsheet (Figure 5.32), the overhead of the first column was totally condensed and the lights were distilled off in the second column. The first column was running at a lower pressure compared with the second column in order to achieve a lower bottom temperature that would prevent a reactive chemical problem occurring in the bottom of the first column. Under these conditions, the lights could no longer be condensed at an acceptable temperature level.

In the alternative flowsheet (Figure 5.33), the first column is operating with a partial condenser. To satisfy the constraint of the bottom temperature, the bottom concentration is allowing some lighter product to lower the temperature. These lights are removed in the last column, which is designed as a divided wall column. This is a typical example of how a heating-cooling-heating sequence (do-undo-redo) can be avoided.

The above discussion has focused on the lowering of energy targets, as this creates the major opportunities. However, clever energy integration to design an optimal energy network is seen as a basic design activity.

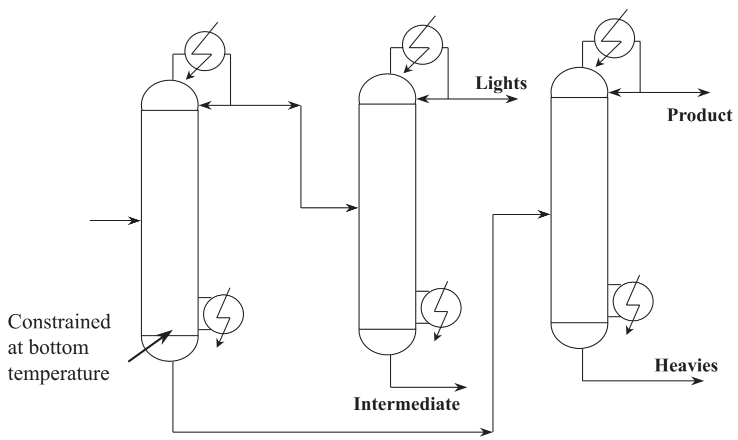


Fig. 5.32. Original flow sheet.

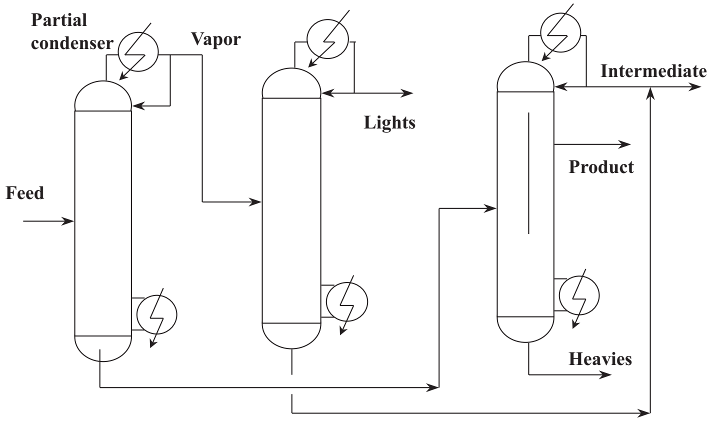


Fig. 5.33. Energy savings realized by partial condenser on overhead of first tower, bottom temperature constraint is removed by allowing intermediates in bottom, and side stream on the last column.

5.6.2
Single Train Design

The design of single trains offers a major opportunity to save not only on capital but also on operational costs. The problem is that all types of restrictions are involved, and the scale-up of a unit or systems will invariably be discouraged by people who are not directly involved with the process. Here, we will restrict the problem to the technical arguments. The most important technical factors that set constraints on a design have been described earlier (see Section 4.2.1.3 in **Chapter 4**), but are outlined briefly-at this point:

- Mechanical design
- Mechanical construction
- Flow distribution and mixing
- Process design
- Combination of mechanical and process design

Mechanical designs need to be sufficiently resistant against thermal chocks. This requires an improved operation to reduce thermal chocks, or the development of a more flexible mechanical design. Different constructions might be applied for equipment and piping to cope with temperature excursions. An example is the application of a high-temperature heat exchanger that is subject to large temperature excursions. In this case, a conventional shell and tube exchanger might be replaced by a hairpin or bayonet-type exchanger (Figure 5.34). The transition from a flue-gas-heated tubular reactor to a radial reactor was described earlier (Figure 4.10 in **Chapter 4**). Mechanical loads might also be reduced by using a lower-weight material with higher strength, or by the application of spring-loaded supports to reduce mechanical forces.

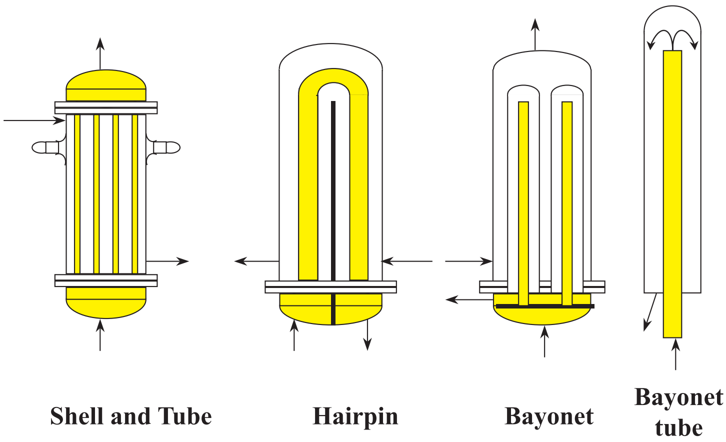


Fig. 5.34. Heat exchangers with increasing flexibility for temperature excursions from left to right.

Mechanical construction might be limited by the furnaces available for heat treatment, such as glass-lined. During the past few decades the size of glass-lined vessels has increased from 20 m^3 to over 60 m^3, and this might increase further still in future. Shop versus field fabrication, which often depends on transportation restrictions, may also have an impact on size.

Flow distribution and mixing is a factor that is considered to be one of the most difficult points for scale-up. In the meantime, wide application of computational fluid dynamics (CFD), which also has the capability of including reaction kinetics, has greatly reduced the risks associated with scale-up.

Process design constraints might also appear, an example being the STR that is constrained by a jacket cooling a solution, and which might be a refluxing condenser (Figure 4.11 in **Chapter 4**). Combinations of mechanical and process constraints might also become apparent. One solution to this was found by modifying a nitration reactor system of CSTRs in series (which is completely glass-lined) by using an adiabatic plug flow reactor system (Figure 4.8 in **Chapter 4**).

Although many systems might be considered as being constrained, careful study of these constraints might lead to solutions of the problems involved. The accompanying savings in costs are extensive, and clearly worth the effort.

5.6.3
Strategy Around Supplies and Storage

Flowsheets of the evolution of batch processes (Figures 1.4–1.7 in **Chapter 1**) show that, by the second millenium, the latest generation of systems were using additives prepared by suppliers and delivered in containers, rather than prepare additives on-site. This avoids the handling and storage of large amounts of chemicals, and hence the process is made much safer and cheaper to operate. For some utility systems, such as cooling water, the addition of chemicals is placed in the hands of specialized companies who supply, operate, and service these systems. This keeps the operators' hands free to carry out more direct, process-related activities.

Utility supplies represent another area where outside companies have taken over the ownership, operation and service. Supplies such as cooling water, steam, air, nitrogen, and refrigeration are added to the historical supply of electricity, gas, and water. These activities will also unload process operation from their primary task. Such supplies can be cheaper and more reliable than on-site generation, because the suppliers of the utilities are experienced in this field, and often operate standardized units remotely. It is in their benefit to keep their prices competitive, and to maintain availability and reliability. In particular, it is the standardization and robustness of these designs, next to the capability of monitoring and operating them remotely, that makes this approach a realistic option.

Care should be taken that contracts cover not only capital, operational costs and service costs, but also guarantee availability and reliability. These guarantees should include the total planned and unplanned outages in time, and also include penalties for contract violations.

Optimization of storage areas is a very important point due to the high fixed and operational capital involved. Storage optimization must be done in concert with the whole supply chain. In these studies, the option for zero storage by using pipeline and/or transport containers needs to be part of the study, and the batch process shown in Figure 1.4 of **Chapter 1** is an example of this. The optimization techniques for sizing the storage are discussed in **Chapter 9**, and are based on probability analysis of supply, demand, and operation performance.

5.6.4
Strategy Around Single Component Design

This point was referred to during the description of the design philosophies. It is, however, a general point for the process designer to consider, and will be discussed in greater detail in **Chapter 6**.

Summary

Process simplification is explained with reference to different categories, all of which should focus on the objective of more economic designs.

- The avoidance of equipment plays a dominant role, and in this respect one might consider in line with Trevor. Kletz's statement: "*what does not exist can't leak and does not cost anything*".
– Avoiding equipment can be realized by critically reviewing the functional need and added value of that equipment.
– Tanks and vessels are a primary target for elimination or reduction.
– In current designs, transport of fluids only very rarely benefits from forces of gravity or pressure.
– Recovery systems in a well-designed process should be nonexistent.

- Do-undo-redo activities result in additional equipment that might be subject to removal.
- Multiple trains and spare installed equipment offer major opportunities for avoidance, and should receive close attention.

- The combination of process functions offers major possibilities for simplification.

- The combination of reaction and separation opens opportunities to increase conversion by shifting the equilibrium and increasing selectivity, at lower investment. Reactive separation examples include: reactive distillation, reactive extrusion, reactive extraction, reactive absorption, reactive adsorption.
- The combination of distillation separations offers advantages through more extensive application of dephlegmators, side streams, and divided wall columns; this results in fewer separation columns.
- The direct coupling of distillation columns can also be exploited around reactor system where the conversion is limited.
- The combination of different separations such as: extraction where more extractions can be executed in one column as neutralization and washing; absorption and stripping; devolatilization and evaporation; stripping and blending extrusion.

- Integration of equipment is another level of simplification. The benefits of this are often less than derived from the integration of functions, but they might be substantial on equipment costs and piping. Several examples are given for the integration of reactor systems. The integration of distillation equipment also receives wider application, resulting in lower capital costs; similar opportunities are also exploitable with other units.
- Intensification of process functions; progress made in this area can be divided into three categories:

- Building more compact units by installing more area per unit volume. Compact heat exchangers are well known in this area. Also, mass exchangers based on separation membranes (e.g., reverse-osmosis and ultrafiltration), as well as gas absorption through membranes are being developed.
- Increase heat, mass and impulse transport. In many heterogeneous reactions the conversion rate is limited by mass and/or heat transport. In these situations, intensification is highly beneficial. Different techniques are applied to enhance transport, such as intensive mixing and re-mixing of liquid/liquid reaction medium, intensified mixing of gas/liquid, application of pulsing flow techniques to create large surface area, and surface renewal in trickle flow reactors.
- Benefits from centrifugal fields ("Higee"). The exploration of centrifugal forces to improve phase separation and allow for higher processing velocities was initially not successful, the development time being much longer than expected. However, industrial applications of "Higee" technology are increasing, and include: de-aeration (devolatilization) of liquid streams; rotational particle separation for sizes >0.1 μm in dust and mist streams; reactive stripping in a rotating packed bed; polymer de-volatilization and pelletization in rotating packed beds.

- Overall process simplification is based on critical review of the overall process functions to identify areas for elimination and combination by modification of the process flowsheet structurally. Areas for consideration are:
  - Design for 100% conversion does not require expensive recycle systems.
  - Critical review of all additives to prevent expensive recovery and destruction sections.
  - Prevention of waste streams does not require waste treatment facilities.
  - Adiabatic reactor operation might result in lower capital and lower energy consumption.
  - Combination and coupling of functions is an essential part of simplification.
  - Energy integration of units needs to apply exergy and pinch analysis for heat exchanger network design, but reduction of the energy targets is the first priority.
  - Implementation of energy networks should follow the basis implementation rules:
    (i) Apply process integration in the following order of priority: unit, section , process, site (complex).
    (ii) Apply heat exchange between flows of similar heat capacity (mass flow times specific heat).
  - Design of a single train versus multiple trains creates large capital benefits.
  - Externally supplied services do not require capital, and also avoid operation and maintenance activities for the organization.
  - Redundant provisions versus reliable robust designs points to single equipment.

These approaches have led to major successes.

5.7 Simplification and Ranking per Unit Operation

The first sections of this chapter have focused on the techniques of achieving simple and robust process designs, and incorporated the following categories:

- Avoidance or elimination of process functions.
- Combination of process functions.
- Integration of equipment.
- Intensification of process functions.
- Overall process simplification.

In the following sections, an alternative approach is taken, and opportunities for the simple and robust design of specific units will be discussed. These include:

- Reactors
- Distillation and absorption
- Extraction
- Adsorption

- Heat exchange
- Fluid transport
- Piping
- Instruments

The objective of this section is to create a list of increasing complexity for several of the most common units operations. Piping and instrumentation are also discussed to illustrate how problems of complexity can be approached for these items. The selected unit operations will be ranked in order of their increasing complexity. It is not the intention here to develop a design methodology for these items, but to use it as a reference of what is "simple", and what effect increases in complexity can have on the design. The priority ranking is based on industrial experience but it always has to be judged in the context of the specific situation. Often, designs are initially too complicated because they are based on the engineer's personal experiences. Design engineers must realize that there are simple ways of doing things, and that the priority ranking applied to the different items is intended to promote simple thought processes. The innovative techniques are not included in the listing, neither is it the intention to list items that have a multiple function. However, these are included in the ranking as they might be used for a mono function as well as multiple functions. In this respect, it should be understood that a mono function such as reaction and absorption includes the inherent heat transfer system to remove reaction or absorption heat, as is applied in multi-tubular reactors. However, reactor feed effluent heat exchange in a reverse-flow reactor and reactive separations as reactive distillation are considered as being multi-functional.

Piping and *instruments* have been included as these have a considerable impact on complexity, specifically for operations. The terms contributing to complexity as presented in Section 2.2 in **Chapter 2** come within the context of piping and instruments, and are re-discussed in this section.

5.7.1
Reactors

Reactors are the most important part of a process as they are the place where the products are formed and the selectivities are determined. Reactors are where the energy "household" requires adequate design and control, and where safety aspects must be respected. In this section, the discussion will be restricted to continuous reactors, (Krishna and Sie, 1994; de Hooge and de Nobel, 1998) which can be divided into the following categories:

1. Homogeneous reaction, G and L
2. Heterogeneous, L/L
3. Heterogeneous reaction, G/S and L/S
4. Heterogeneous reaction, G/L
5. Heterogeneous reaction, G/L/S

The status of knowledge at any one time determines into which category the reactor design will fall. Thus, the selection of category is seldom an option at the design stage, but will be made at the research stage, when three general rules to simplify the development must be followed:

1 → Reactions within a gas phase should, preferably, be converted to liquid phase reactions, the advantages of which include:

- better mixing;
- higher concentrations;
- easier heat conditioning; and
- smaller equipment dimensions.

An exception is that of reactions which take place inside the catalyst particle, where diffusion plays an important role. In such cases, the high diffusion coefficients of gases offer a major advantage.

2 → Heterogeneous reactions should, preferably, be converted to one phase, either liquid or gas. The advantages of homogenous reactions are:

- no mass and heat transfer limitation between phases; and
- flow conditions are more easily implemented.

This also explains why reactor intensification concentrates on heterogeneous reactor systems, to minimize these limitations (see Section 5.5).

3 → Integration of multiple functions in one reactor system should also be considered as an option, especially for equilibrium reactions, where shifting of the reaction will lead to higher conversions and selectivities (see Section 5.3.1)

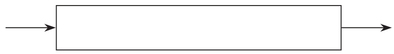
The *reactor category* is predetermined at the design stage, and will fall into one of the above categories. The macro design of the reactor within the selected category will be determined by:

- catalyst selection;
- energy household; and/or
- mixing/flow distribution.

For priority ranking in terms of simplicity of the different categories, the chemistry (as well as the catalyst selection) is beyond this discussion. However, the types of reactor employed in the different categories will be discussed briefly, and a priority ranking will be made. In the examples given, the related heat transfer is seen as heat removal, although it is also applicable to heat addition (in which case the terminology must be adapted).

5.7.1.1 Homogeneous reaction; G and L

Tubular reactor The most simple form of a reactor design is a tubular reactor. Here, the only provision that needs to be added is the heat transfer.

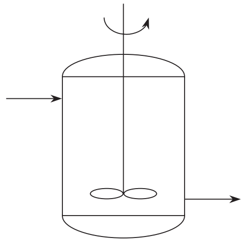


Tubular reactor

The heat transfer alternatives are included at an increasing level of complexity. An adiabatic design for endothermal, as well as exothermal reactions, is – in its simplest form – an empty tube.

- The way that the adiabatic condition is realized is also ordered in terms of simplicity, and in order to discuss this more fully we need to refer to exothermal reactions:
  - Increase in process flow by either one of the reactants.
  - Increase in solvent flow, although this will result in lower concentrations of the reactants.
  - Decrease in inlet temperature of the feed stream; this might be limited by the start temperature of the reaction. In the reactor presented in Figure 4.7 in **Chapter 4**, this was elegantly solved by creating an adiabatic CSTR in front of the tubular reactor, all in one embodiment. In this way the temperature in the CSTR is maintained well above the start temperature while the inlet temperature can be lower.
  - Injection of cold feed is an other option (see Figure 5.26, which describes a tubular reactor for the peroxide production using the anthraquinone route). This latter option is more difficult to operate, and requires a sophisticated automated control design, (Tururen et al., 1999).
  - A combination of the above-mentioned options.
- Heat exchange with the reactor: here, different designs are available, and although the application depends heavily on the specific reaction, the designs include:
  - jacket pipe, for tubes;
  - a staged, inter-cooled reactor system; and
  - a shell and tube-type of reactor.

Continuous stirred tank reactor (CSTR) The CSTR for homogeneous reactions is the second best with regard to simplicity of design. This type of reactor needs to condition mixing and heat transfer.



Continuous Stirred Tank Reactor

Heat transfer is ranked in terms of increasing complexity for exothermal systems:

1. Increase process flow and decrease inlet temperature, as discussed under the plug flow reactor.
2. Reflux condenser applicable for boiling systems.
3. Internal cooling with spirals (fouling might cause a problem).
4. Jacket cooling of most standard reactors can be provided with jackets, though scale-up may be difficult at the same length to diameter (L/D) ratio; this is because the volume increases with cube of the diameter (D^3), while the surface increases with the square (D^2).
5. External cooling through a recycle.

Mixing is seldom a problem for a homogeneous liquid system, but this is not to relevant to this discussion.

The ranking of the alternatives with increasing complexity lists as follows:

1. A jet mixer for the inlet stream; in the case of jacket or internal cooling, this might limit the heat transfer. To create overall mixing, careful design with a CFD code is a requirement (specifically for gas reactors).
2. An agitator is often used to enhance heat transfer device, especially in combination with a jacket or an internal coil. One drawback, however, is that agitators require more power and maintenance.
3. In a recycle system, a jet mixer is often used in combination with an external heat exchanger; in this case the circulation pump is in shared service.

5.7.1.2 Heterogeneous reactions; L/L

These reactor designs follow the same order in priority as the homogeneous reaction. The difference is made by the mixing. Indeed, it might be said that stirred tank reactors have bad mixing and mass transfer properties for two-phase systems (as discussed earlier in Section 5.5.2; see also Figure 4.8 **Chapter 4**). When the reaction is transferred from a CSTR to a plug flow reactor, the ranking order will be:

1. Plug flow reactor provided with mixing elements and re-mixing elements in order to achieve high mass transfer rates.
2. CSTR provided with high-efficiency mixing.

5.7.1.3 Heterogeneous reactions: G/S and L/S

Fixed bed and fluidized beds are the main reactor types selected for this category. The fixed catalyst beds are mostly operated with top-to-bottom flow (to avoid fluidizing), and consist of large particle sizes. The opposite is true for fluidized beds: the flow is upward, while the catalyst particles are small in order to accommodate the fluidized state. The fluidized beds are selected for systems which need high-frequency regeneration of the catalyst, and where the uniformity of temperature is a stringent requirement, for example temperature-sensitive reactions. In some applications the fluidized bed is used in homogeneous reactions simply to control the temperature; examples are the chlorination of hydrocarbons or the oxidation of gaseous fuels. The ranking of reactor types with increasing complexity is as follows:

1. Adiabatic packed bed; this is the cheapest type, and is mainly restricted by energy transfer requirements.
2. Packed bed with cooling requirements; cooling may be provided in several ways:
   - Recycling of cooled, unconverted reactant or solvent (this makes it an adiabatic bed).
   - Cooling through intermediate injection of cold feed or solvent.
   - Multi-stage beds with inter-stage cooling; these beds are often designed as radial beds for high-capacity operations (e.g., NH_3 reactors and ethyl-benzene de-hydrogenation). These beds may be built as a single embodiment.
3. Fluidized bed:
   - With solids removal through the wall; this is applicable when the velocity selected does not bring the fluid particles in the dilute phase.
   - With solids removal through internal cyclones; this is applicable for high-velocity systems to keep the solids in the fluidized bed.
   - With solid removal through external cyclones, specifically if cooling is provided through recycling of the solid stream.
4. Multi-stage fluidized beds are used for: Catalytic reactions where a high conversion is required, and which must be satisfied through plug flow and suppression of by-passing; gas solid reactions or solid reactions (e.g., the calcination of lime). In this last application, different functions are combined in order of processing of the solids: preheating and drying stages (to be seen as a countercurrent heat exchanger with the flue gases); calcination stage followed by cooling stages utilized for air preheating (see Figure 5.18). Any imbalance in the heat recovery is often utilized for steam generation.
5. Multi tubular reactor applied to highly exothermal reactions such as oxidation or hydrogenation reactions. The heat removal is performed respectively with:

- boiling liquid, such as water in a thermo-syphon design. In some applications this is done with different boiling zones, which adds to the complexity; and/or
- circulating liquid, such as molten salt for high-temperature applications (e.g., dehydrogenation of ethyl benzene).

5.7.1.4 **Heterogeneous; G/L**

For heterogeneous G/L reactor systems, several very different forms are possible. Especially important in the design of the system is the volumetric ratio of gas versus liquid. Fundamentally, there are three different modes of gas liquid contact to be recognized:

1. Gas bubbles dispersed in liquid, as in bubble columns.
2. Liquid dispersed in gas, as in spray columns.
3. Gas and liquid in film contact, as in packed columns.

A selection criterion, β, is the ratio of the liquid volume to the volume of the diffusion layer within the liquid phase (Krishna and Sie, 1994):

$$\beta = \frac{\varepsilon_l}{\delta_l a}$$

where ε_l is the fractional hold-up of the liquid phase, a is the interfacial area per unit volume, m^{-1},

δ_l = thickness of diffusion layer of liquid phase $\delta_l = \frac{D_l}{k_l} \cdot m$

where D_l is liquid diffusion coefficient $m^2\ sec^{-1}$ and k_l is liquid phase mass transfer coefficient $m\ sec^{-1}$.

For gas bubbles dispersed in the liquid phase, $\beta = 10^3$–10^4, while for gas in liquid film contact and the liquid dispersed in gas, β = 10–40. The overall aim is to choose the value of β such that the reactor volume is effectively utilized.

For slow, liquid-phase reactions the liquid phase volume is increased at the expense of the interfacial area. A high value of β is achieved in bubble columns and tray columns operating in the froth regime, occasionally with higher weir heights to increase the liquid hold-up on the trays. An example of the bubble regime application is wet air oxidation, it might also be used in biological aeration basins and fermentation reactors. The HNO_3 and H_2SO_4 absorption towers are other typical applications in this field where the hold-up is increased by application of excessive high weirs heights; it should be noted that in these cases the heat removal is extensive and is carried out on the trays with cooling spirals.

For rapid reactions, the reaction is mainly limited to the diffusion layer, and low β values are preferred (spray columns and packed columns). The aim is to increase the interfacial area, but there is no need to overemphasize turbulence in the liquid phase. The absorption of CO_2 in caustic solution is carried out in packed columns.

Within the consideration of the above discussion, the following ranking is selected respectively for slow reactions which take place in the liquid phase (liquid phase-controlled), and for rapid reactions which take place at the interface (interfacial-controlled).

Liquid phase-controlled reactions

These include:

1. Bubble column
2. STR with jet mixer
3. STR with agitator with gas dispersion in the liquid
4. Multi-tray bubble column (the liquid is the continuous phase)
5. Tray column (the gas is the continuous phase)
6. Membrane gas absorption; this technique is ranked at the bottom of the list, but it might develop into a recognized separation system as an increasing number of industrial applications are installed.

Interfacial-controlled reactions

These include:

1. Spray column
2. Packed column

5.7.1.5 Heterogeneous; G/L/S

These types of reactors are mainly applied where gas liquid reactions are supported by a solid catalyst, as in hydrogenations. From a transfer-reaction perspective, the choice must be made between a small catalyst particle and catalyst pellets or extrudates.

The small catalyst particles (<1 mm), as applied in slurry reactors, require an expensive recovery system and therefore are not considered high priority here. In the case of high heat releases, this approach may be more favorable over multi-tubular reactors when the reaction temperature is controlled by evaporation.

The priorities are ranked as:

1. Trickle flow, packed bed reactors
2. Packed spray columns
3. Packed bubble column
4. Slurry reactor
5. Multi-tubular reactor

Heat transfer may dominate the final design. The preferred technique always supports adiabatic operation before any external heat transfer device with the reactor is considered The preferred options are as mentioned previously:

- Increased flow of unconverted reactants or solvent.
- Decreased inlet temperature or application of distributed cold injection of feed.
- Evaporation of reaction medium.
- Heat exchange within the reactor.

Reactor devices will always be a balance between thermodynamic equilibrium, reaction kinetics, and heat and mass transfer, complemented with a desired flow pattern. This must all be encapsulated in a cost-effective manner. The above-mentioned information was provided to help the designer stay on a simple track. It was not the intention to cover all reactor types, but more to install a thought process that might not be encountered in design manuals. The results are summarized in Tables 5.7 and 5.8.

Summary

As there is a large differentiation in types of reactors they have to be divided into categories. The most practical and accepted method is by differentiation of the phases involved. The first split is made between homogeneous and heterogeneous systems while heterogeneous reactor systems are further split in: L/L, G/L, L/S, G/L, G/L/S.

The selection of preferable reactor types was made in a generic way independent from thermodynamics or kinetics consideration which always will put constraints on the reactor system design as does the availability of the specific reactor technology.

Table 5.7. Summary of reactor systems, homogeneous G and L and heterogeneous L/L, the ranking of reactor selection in order of increasing complexity.

Homogeneous G and L	*Options for cooling*	*Options for mixing*	*Heterogeneous L/L*
1) Adiabatic tube			1) Adiabatic tube
	a) Process flow, up	Static mixers / vortex mixers	
	b) Solvent/heat carrier, up		
	c) Inlet temperature down		
	d) Cold feed injection		
2) Tube(s) with heat exchange			
	a) Jacket pipe		
	b) Staged inter-cooled		
	c) Shell and tube		
3) CSTR			2) CSTRs in series
	a)Process flow, up	a) Jet mixer with feed/ agitator	
	b) Reflux condenser	b) Jet mixer with feed/ agitator	
	c) Spiral cooling	c) Agitator	
	d) Jacket cooling	c) Agitator	
	e) External cooling	c) Jet mixer with recycle	

Table 5.8. Summary of heterogeneous reactor systems G/S and L/S, G/L, G/L/S the ranking of reactor selection in order of increasing complexity.

G/S and G/L	*G/L*	*G/L*	*G/L/S*
	Liquid phase controlled	Interfacial controlled	
1) Adiabatic packed bed	1) Bubble column	1) Spray column	1) Trickle flow packed bed
2) Packed bed(s) with cooling a) recycle b) cold injection c) inter-stage cooling	2) CSTR, jet mixer	2) Packed column	2) Spray column packed bed
3) Fluidized bed	3) CSTR with agitator		3) Packed bubble/ multi-stage, column
4) Multi-stage fluidized beds	4) Multi-tray bubble column		4) Slurry
5) Multi-tubular reactor	5) Tray column 6) Membrane separation		5) Multi tubular

The *general rules* for the design of reactor systems to obtain less complex systems are:

1. Design for homogeneous liquid phase reactor systems, the liquid phase is preferred above the gas phase.
2. Heterogeneous reactor systems are preferably converted to homogeneous systems.
3. Integrate reaction with other process functions like: other reactions, distillation, extrusion, heat exchange (reverse flow reactor).
4. Reactor systems are preferably operated adiabatic (no heat transfer provisions), with larger solid particles (easily captured/separated), flow distribution/mixing by static devices.

The ranked reactor types with an increase in complexity did not take into account any thermodynamic or reaction kinetics information which might force the designer from an economical perspective to a more complex reactor design. The results of the reactor discussion are summarized in Tables 5.7 and 5.8.

5.7.2
Distillation and Absorption

Distillation and absorption is one of the oldest – and certainly one of the most applied – separation techniques used for homogeneous mixtures. The advantage is that it can easily be designed based on vapor liquid equilibrium data that are readily available in public databanks, or can be determined at laboratory scale at relative low cost. Another advantage is that this technique is able to provide sharp separations, as long as there is a reasonable difference in volatility. The risk concerning the design of distillation systems is rather low, and also impacts upon the development track of new processes. The disadvantages include the high capital cost involved, and also the high related energy costs.

Despite distillation and absorption being available for more than a century, only during the past few decades have considerable improvements been made in this process. The drive behind these developments has, in the main, been the energy crises, in addition to new-found capabilities of modeling complex systems, both statically and dynamically. These improvements have resulted in:

- the large-scale application of packed towers;
- improved packing performance, and the wide application of gauze and sheet packing;
- reactive distillation applications; and
- divided wall column applications (three-component separation) (Kaibel, 1987; Triantafafyllou and Smith, 1992; Lestak and Smith, 1993; Mutalib, 1995).

Despite such rapid advances, only the first two developments mentioned have been applied more widely. Reactive distillation has been introduced to a degree, but is limited to only a few specific applications, while divided wall columns are only just beginning to be implemented in some broader area.

The development of flowsheets (see Figures 4.16–4.20 in **Chapter 4**) taught us how much can be saved by combining the different distillation set-ups. Nonetheless, it might be considered remarkable how seldom designers deviate from sequential distillations of two-component separations, and this concept has formed the basis behind the listing of these techniques as:

- One- and two-component separation
- Three-component separation
- Four-component separation

One- and two-components separations are ranked in order of their increasing complexity (Figures 5.35 and 5.36):

1. A *flash* is the most simple form of vapor liquid separation, where the vapor is enriched with the most volatile component.
2. A *stripper column* takes care of the purification of a liquid stream by removing volatile components by a vapor stream.
3. A stripper column is applied for the purification of a liquid stream where the overhead forms an heterogeneous azeotrope, which after condensing separates into two liquid phases. The component to be removed from the feed leaves the system, while the remaining stream is applied as reflux. Water purification from dissolved hydrocarbons is a very common application for this type of stripper. The method can be applied to minimum boiling heterogeneous azeotrope removal.

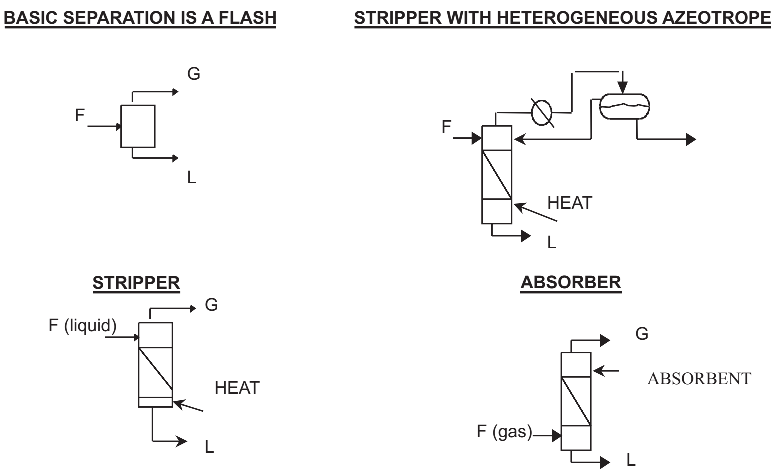


Fig. 5.35. Flash, Stripper, Stripper with heterogeneous azeotrope, Absorber.

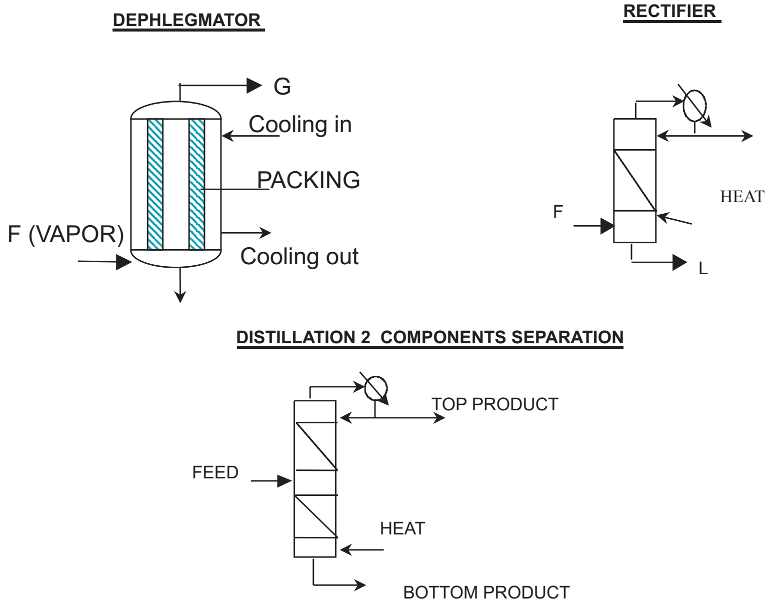


Fig. 5.36. Dephlegmator, Rectifier, Distillation column.

4. An *absorber column* is used to purify a gas stream by absorption of the least volatile component in a solvent. Often, the absorption is achieved by chemical reaction compared with physical absorption, such as the removal of CO_2 or H_2S.
5. A *dephlegmator* is a nonadiabatic rectifier, where a vapor stream is purified by partial condensation of the vapor in a rectification section and refluxed.
6. A *rectifier column* purifies a vapor stream by partially condensing and refluxing the overhead on the top of the separation column (a specific form of dephlegmator).
7. Two-component separation in a standard distillation column.

Three-component separations are ranked and presented in Figure 5.37.

1. A *distillation column* with a vent stream with lights removed at the top, a top liquid product and a bottom stream (in case the light stream would not be pure enough, a dephlegmator might be installed at the vent).

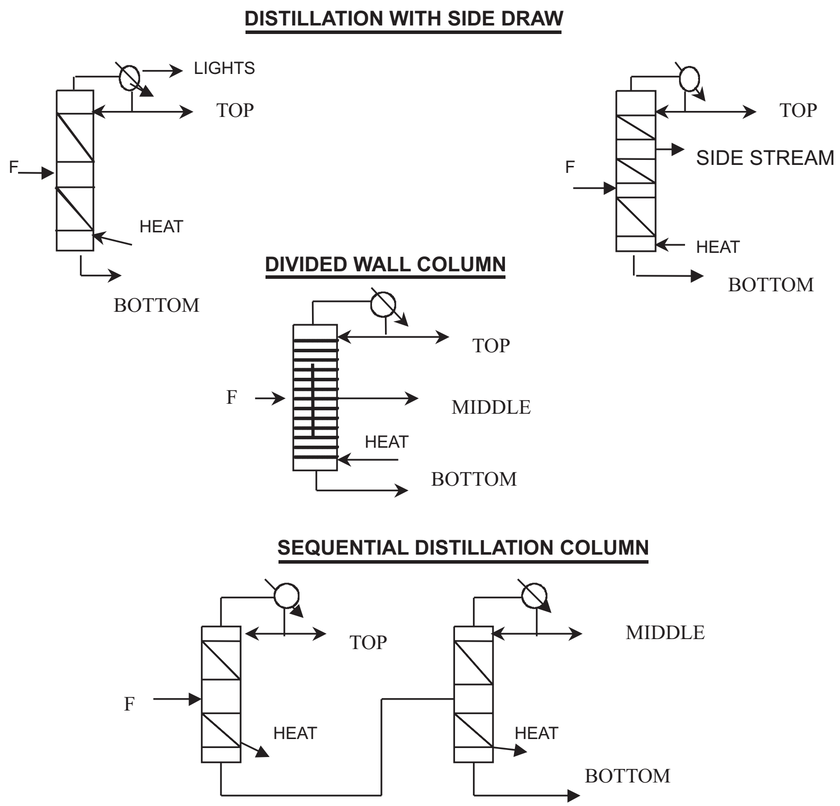


Fig. 5.37. Three component distillation with; side draw, divided wall column, two sequential columns.

2. A distillation column with a side stream as a third product stream.
3. A distillation column with a purified side stream with either a side stripper or a dephlegmator or rectifier – installation of a side stripper or rectifier within the column is a prefered option (Figures 5.4 and 5.5).
4. A *divided wall column* with a purified side stream.
5. Direct coupled column (see Figures 5.10 through 5.13).
6. A sequence of two distillation columns.

The above alternatives for one-, two-, and three-component separation are summarized in Table 5.2.

Four-component separations are listed in order of increasing complexity are shown in Figures 5.38 and 5.39:

1. A distillation column with lights removed at the overhead condenser, liquid top product, side product stream, bottom stream. (lights might be purified further with a dephlegmator at the top).
2. A distillation column with lights removed at the overhead condenser, liquid top product, purified side product stream, bottom stream. (purification of side draw with either a side stripper or a dephlegmator).
3. A divided wall column (DWC)with lights removed at the overhead, liquid top product removal, side product streams, bottom stream.
4. A divided wall column with two side streams as third and fourth streams.
5. A divided wall column followed by a conventional distillation.

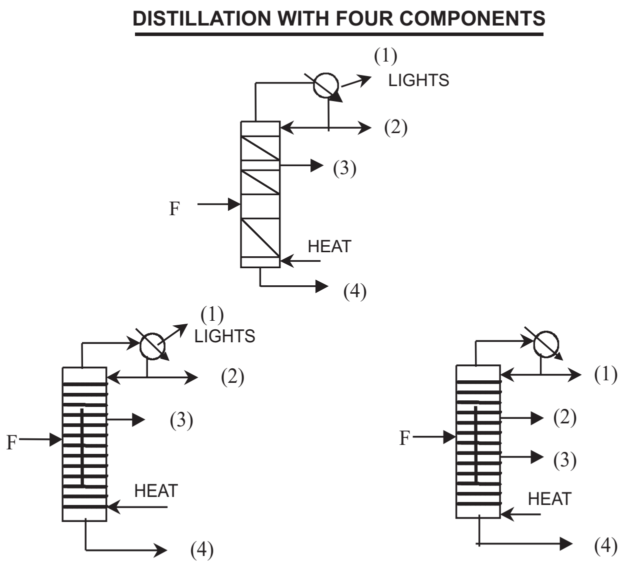


Fig. 5.38. Four component separation with; side draws or DWC

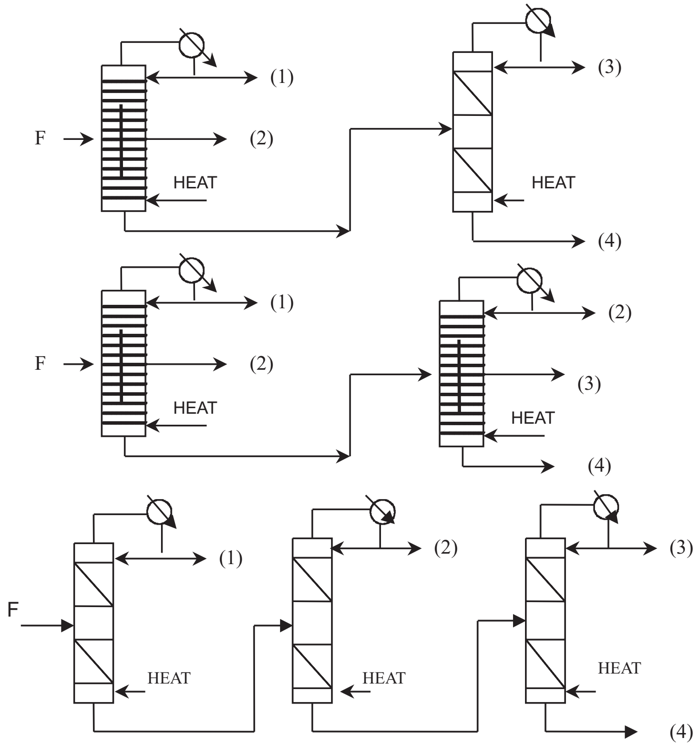


Fig. 5.39. Four component separation with; one DWC and a sequential column, two DWC's or three sequential columns.

6. Two divided wall columns where product 2 is removed as a side stream of the DWC and at the top of the second column. This application is chosen when the temperature range over the first DWC would be too large; then, some product 2 is left in the bottom to lower the temperature. A similar approach was applied for the installation of a partial condenser (see Figure 5.33).
7. A sequence of three distillation columns.

An overview is given of the one-, two-, three-, and four-component separations in order of complexity in Table 5.9. It is clear that the conventional approach of distillation columns in series is more complex and more expensive as an increasing number of columns becomes involved.

Most *absorption units* are based on chemical absorption versus physical absorption. The standard physical absorption unit is a packed or tray column. The chemical absorption units were discussed in the section on G/L reactors.

The above illustrates that many options exist for multi-component distillation separations before a selection ends in a conventional approach with standard distillation columns in sequence. It might be considered surprising that, despite these

Table 5.9. Distillation for one, two and three purified streams in order of increasing complexity.

Distillation	*No. of purified streams*
Flash	0
Stripper	1
Absorber	1
Dephlegmator	1
Simple distillation	2
Distillation with side draw	2 pure, 1 impure
Distillation with purified side draw (side stripper or dephlegmator/rectifier)	3
Divided wall column	3
Direct coupled distillation	3
Distillation with lights, top, side and bottom streams	4
Distillation with lights, top, purified side draw, bottom streams	4
Divided wall column lights, top, side and bottom streams	4
Divided wall column top, two side and bottom streams	4
Divided wall column and a distillation column	4
Two divided wall columns in series	4
Three distillation columns in series	4

available techniques, engineers still select the conventional approach of a series of normal distillation columns. The only answer to this problem is *conservatism*.

5.7.3
Liquid–Liquid Extraction

Extraction is also a very old technique used to isolate a component from a homogeneous mixture. The differences in distribution coefficient of the components within the solvent determines the separation. The solubility of the solvent in the raffinate is preferably very low. Next to the distribution coefficients, the primary selection criteria for the solvent include differences in density, tendency for emulsion formation, and ease of separation of the extracted component. All types of process industries utilize this technique, ranging from pharmaceuticals to food and fine chemicals. In the pharmaceutical and fine chemical industries the quantities of material involved are often relatively small, and this impacts upon the selection of equipment. In these areas, batch extraction is quite often applied, using standard equipment such as stirred tank reactors that are already being used for other steps in the production. In this situation, *settling*, which is inherent to liquid-liquid extraction, is carried out in the same vessel, as a batch-wise operation

The priority ranking for continuous operations is affected by the number of stages required, as more stages require less solvent for processing. The selection of the continuous phase is a choice to be made that can have a major impact on the performance of continuous operations. In particular, the density gradient over the continuous phase will support or depress any overall circulation in this phase.

The simplest extraction will be one stage, and therefore start the ranking:

1. One-stage mixer settler; here, the mixer is selected as a static mixer, being the simplest component. On occasion, rotating mixers are used, but these are mainly applicable at large flow variations. In that respect, a pump is not a very good mixer as it is not designed for that purpose. The settlers selected will be gravity-based, and provided with additional surface area by the installation of separation plates located short distances apart to decrease the settling distance and time (see Figure 5.24). These separation plates also limit any overall circulation that will reduce the performance. A disadvantage of the system is the large hold-up and related residence time.
2. Spray columns are used for larger flow rates, but have the disadvantage of overall circulation. This causes a deterioration in performance such that only one or two theoretical stages are achievable.
3. In packed columns, the packing reduces overall circulation, but in the case of counteracting density differences will not be sufficient.
4. Tray columns.
5. Mechanically agitated columns; several alternatives have been developed over the years, but with limited performance differences. Included among these are rotating disc columns, the Kühni column with rotating impellers, and Karr columns provide with reciprocating vertical displacement of stacked discs.
6. Pulsing columns; the feature is a reciprocating device like a piston or membrane, which moves the liquid to enhance mass transfer. This is often implemented as an additional device to a packed or tray column.
7. Centrifugal extractors (Podbielniak extractors are a specific alternative); these are intensified units with multi-stage performance. They are useful for small density differences, and have little hold-up.

Note: multiple stage mixer settlers have been eliminated as being a bad choice.

5.7.4
Adsorption/Chemisorption

Adsorption is performed, as a first choice, batch-wise in fixed beds, and two parallel beds are often installed for alternate use during regeneration. The benefits of this approach are the ease of operation and robustness in performance. Regeneration makes this operation rather expensive, as either aggressive chemicals as used for ion-exchange applications or conditions of extreme temperature and/or pressure are required. The most common application are ion-exchange units for water treatment. New techniques have been developed to reduce the size and ease of regeneration. This technique is based on frequent switching (within minutes) between adsorption and de-pressurized desorption (regeneration). By doing so, the heat of adsorption is available for desorption. This technique of high-frequency pressure swing adsorption (PSA) is applied for air purification. The desorption is carried out by depressurizing the system to vacuum, and has as an advantage that the bed size is largely reduced. This in comparison with temperature swing absorption, which requires a longer cycle time. An alternative adsorption system in use for hydrogen purification is based on a simulated moving bed. A number of beds in series is changed during service in a planned manner to simulate a continuous adsorption unit, with desorption being instigated by depressurizing. The design of a special multi-port valve has made this technique highly successful.

The design of a real, continuous adsorption system has found little application, mainly because problems with solid handling were not solved adequately.

The order of ranking with increasing complexity has the following appearance:

1. Mixed ion-exchange beds to accommodate simultaneous removal of anions and cations.
2. A high-frequency, alternating operation of absorption, desorption cycle by depressurizing (PSA) is applicable only to gas systems.
3. Fixed bed with pressure, temperature or concentration desorption.
4. Simulated moving bed adsorption.

5.7.5 Heat Exchange

Heat exchange is one of the main supporting units for reaction and separation systems, and developments have concentrated successfully on more compact designs for all types of application. Penetration of heat exchange concepts into the chemical industry – with its conventional shell and tube designs – is still limited compared with that into the food and pharmaceutical industries. However, penetration into the chemical industry will clearly increase as the advantages of high surface-to-volume ratios and more plug flow operation associated with smaller temperature approaches become apparent. The major limitation for chemical systems is fouling, and it is imperative that this has to be solved from the processing point of view. The list of heat exchange systems, in order of increasing complexity, is considered to be:

- Plate fin exchanger
- Plate exchangers
- Jacket pipe and jacket vessel
- Fin tube air coolers
- Hairpin exchanger
- Shell and tube exchangers with;
  - fixed tube sheet
  - floating head
  - bayonet
- Mixed condensers; these are applicable for large quench towers where quench material is kept in a closed system. Such a system still requires a heat exchanger to remove the heat from the quench medium.

5.7.6
Fluid Transport

Fluid transportation needs differentiation in liquid and gas transport, the main difference being the type of mechanical device used – a pump versus a compressor or blower. The types of sealing and bearing will not be discussed at this point. Earlier, we referred to a saying, *"There is no component more reliable than no component"*.

This is specifically applicable to fluid transport, and will be reflected on in the priority ranking. The selection of the different types of machinery is considered a design issue, and is not discussed in this section. The different types of machinery mostly have a specific operational area with some overlap, and can be outlined as:

Liquid transport	*Gas transport*
1. Gravity flow	1. Displacement of liquid
2. Flow through pressure difference	2. Pressure difference by vapor pressure
3. Pump, centrifugal	3. Gas/liquid pump as liquid ring pump
4. Positive displacement pump	4. Fan
	5. Blower
	6. Compressor, centrifugal
	7. Compressor, positive displacement

5.7.7
Piping

Piping may appear simple, but can make the overall process system very complicated. In general, piping networks grow during piping development, usually at the point when the discussion begins regarding "*what if ?*" situations (scenarios).

This always leads to an inventory of possible things that might occur, and which require all types of provisions including cross-connection, bypass provisions, back-up lines, new loading lines, recycle lines – all with their required instrumentation. Subsequently, all of these lines and connections need to explored for potential hazard, through a HAZOP study, which inevitably will add more provisions such as check valves, instruments, and safety devices. This entire situation requires a revised approach to be taken.

An engineer once had to automate a storage area for a plastic plant. The storage contained storage silos in addition to blending hoppers which were provided with material from four production lines and also from several extruder lines applied for product up-grading. At the beginning of the project, he tried to find some logic in the pipe network. The situation was such that nearly all options were available, but most of them were not utilized, and the operator was not even aware of all the options. What the engineer did was to start designing a new piping system as if nothing were available. When he had completed the design, the engineer went into the plant to search for the availability of these lines. His next step was to eliminate all unnecessary connections and lines. Based on the new design, he was able to design software for the storage area.

The objective for piping is *minimize*, as this makes the operation surveyable. This is especially important in remote-operated plants, where the demand for rapid diagnosis of a process upset is high. Next to surveyability, minimization of piping also improves safety, as fewer lines can lead to fewer operational errors. The way that lines are tied together should also be limited, the greater the number of connections, the greater the risk of an inter-reactivity problem.

During the discussion about complexity in **Chapter 2**, the following terms were mentioned with regard to unit complexity:

$$\text{In formula form; C unit} = f\,(\text{M})\ (\text{N})\ (\text{O})\ (\text{P})\ (\text{Q})\ (\text{R}) \qquad (2)$$

The level of complexity C of a unit in a chemical process was defined as a function of:

- M, the number of equipment accessible by the operator.
- N, the number of DOFs, including manual/actuated valves/switches and set points of control loops.
- O, the number of measurement readings.
- P, the number of input and output streams, including energy streams.
- Q, the interaction in the unit requiring an operator intervention.
- R, the number of external disturbances (for the unit) asking for action from an operator.

For piping, this can be transformed in a similar form:

$$\text{Complexity of piping is; C} = f\,(\text{M})\ (\text{N})\ (\text{O})\ (\text{Q}) \qquad (3)$$

where M is number of lines, including bypasses, jump-overs;

N is the number of automatic valves as well as manual, including bypass, drain and vent valves;

O is the number of piping items others than valves, such as check valves, reverse and excess flow valves, safety relieve devices, bellows, excluding reducers (these last are seen as part of the fixed pipe); and

Q is the number of flow interconnections that it is possible to make (see Table 2.1 in **Chapter 2**) if no special provisions are made to avoid any reverse flow.

These terms clearly show how, as the complexity of piping grows, the number of flow interconnections expands exponentially. The solution is clear – the number of piping items shown in Eq. (3) needs to be reduced.

5.7.3.1 **How do we minimize the piping?**

There are several ways to reduce the piping, some being equivalent to minimization of equipment:

- Avoidance of equipment.
- Combination of functions.
- Combination of equipment.

Although all of the above-mentioned actions will reduce piping, it should be realized that in case of the removal of spare installed equipment the removal of piping is more than double the amount of a single unit. Also, the combination of functions and equipment leads to a need for considerably less piping. Recall the situation of when a mixer-settler combination was replaced with an extraction column (see Figures 5.14 and 16), and the comparison of a series of CSTRs versus an adiabatic plugflow reactor (Figure 4.8 in **Chapter 4**).

Specific piping elements which result in the simplification/minimization of piping include:

- Replacement of piping which has many interconnections by a more dedicated line(s). For example, a large manifold might be split into several smaller ones. When a manifold from six connections is split into two manifolds each of three connections, this would reduce the number of flow interconnections from 30, to 2×6 (see Table 2.1 in **Chapter 2**). Minimization of the number of connections is not applicable to utility systems, as in these cases the pressure in the utility system is kept higher than the process operating pressure of the individual users in order to avoid any back flow. If that is not the case, then special precautions must be taken.
- Minimization of piping items. This might seem difficult to instigate, but includes:
  - Bellows; these can be avoided by changing the pipe design.
  - Manually operated bypasses around control or block valves are not preferred when a decision has been made to operate fully automatically. A totally automated process should not be operated on partial manual control, as this will lead to problems.
  - Precision piping bends reduces the need for gasketed and sealed joints, which are the weak points in piping. In high-pressure systems, welding of piping is preferred.
  - ASA flanges are preferred, as these are stronger and provide less chance for leakage at gaskets.
  - Screwed connections should be avoided for chemicals, as they have a greater tendency to leak.
  - Avoid check valves at places where performance on reverse flow is essential, and not simply convenient. In these situations, install positive shut-off valves with back-flow detection. Check valves should be avoided as they are neither reliable nor robust because they are sensitive to fouling and the performance is difficult to monitor.
  - Isolation valves should be carefully selected; too many of these does not add value as such, as they add gaskets to the system, and losses to the environment.

The *"what if ?"* situation (scenario) often results in add-on provisions, and should be addressed in another way during P&ID (process and instrument diagram) reviews. The design philosophies which may be beneficial in such situations are:

- “prevent versus cure”; and
- “first pass prime”.

These are basic approaches to keeping piping designs simple, and when discussions begin about the design of P&IDs, any questions which include the term *“**what if ?**”* should precipitate one of the following responses:
What is the likelihood of this situation?

- What would happen if we did not have the proposed item at that time?
- Could we prevent such a situation, and what would we then need to do?
- If we were to design for first pass prime, would it still be likely to occur?

The operation that should lead to first pass prime operation will be discussed in **Chapter 8**.

5.7.8
Instruments

Instruments are recognized as being the “eyes”, “ears”, and “hands” of the process, and it was during the eighties and nineties that a number of somewhat striking statements came to light:

- A major proportion of the instruments lie or die.
- Instruments are often unreliable during the start up and restart of processes.
- Most process outages are caused by instrument problems.

It is clear that hands-off operation of a simple and robust designed processes, cannot be obtained under these conditions. With respect to instruments, we will here only discuss those issues that are essential for simplification, as instrument design is described in greater detail in Section 8.2 in **Chapter 8**.

From a perspective of simplification, the following design statement should be borne in mind: *“Better a good reliable instrument then lots of unreliable ones”.*

This statement was underlined implicitly by a company which had a large number of remotely operated air separation plants. The company improved operation by eliminating and upgrading instruments on their remotely operated processes, mainly because too many of the instruments did not give the correct information and this led to a great deal of confusion.

In order to simplify instrumentation, it is obvious that by eliminating equipment and combining process functions will result in a need for fewer instruments, in much the same way as was discussed for piping.

The specific instrument elements to achieve simplified instrumentation include:

- Selection of the essential process variables for operation, and their location. Avoid measurements which are only in place to measure equipment performance for the design engineer. *Operation* is the primary purpose of instrumentation – design information can also be measured by clamp-on measurements during test runs.

- Avoid multi-functional debates about what is required – each discipline will want to add instruments that are "nice to have", but not essential for operation.
- Select only reliable and robust instruments to fulfill these requirements
- Avoid the use of "local" instruments. Simple and robust processes have limited field operators. When the local instruments are needed, they often fail or cannot be trusted. Local instrument connections for analyzing operational status at initial start-up and maintenance can be sufficient.
- Avoid instruments with long response times and sample loops. Direct, inline measurements are essential for robustness and adequate control. Long sample lines and lead lines are a source for fouling, and will only cause problems.
- Avoid duplicate measurements, but if these are required for safety or environmental reasons, then install two analog measurements. It is easy for operation and fault detection software to verify which instrument has failed in case of two analog elements.
- Triple instruments are a nightmare and essentially the wrong direction to take. It is better to invest in reliable and robust instruments than in triple redundancy. In specific cases, for instrumental safety protection, there may be no alternative, but always search for better solutions. In the "old" days, it was essential for airplanes to have four engines to fly over the ocean, but nowadays two are sufficient, and the reliability level is the same.
- Avoid manually operated by-passes around control and block valves; a hands-off operated process should not be operated with manual operated bypasses.
- Avoid too many limit switches to verify a process action. For nonfouling systems, block valves should be reliable. Limit switches on these valves add to the unreliability, and are a major cause of nuisance trips. An emergency block valve needs a switch to confirm its emergency action, and not necessarily its stand-by condition. When limit switches are applied they should have a much higher reliability than the valves to be watched.
- The ratio between analog inputs and outputs (AI/AO) and digital inputs and outputs (DI/DO) should be used as a yardstick to compare instrument designs. For continuous processes, an AI/AO a ratio of 1 is the ultimate minimum, but in practice a value of 3 needs to be achieved.

Although simplification is possible by following these guidelines, it is infinitely better to use only single reliable and robust instruments, which are correctly selected, installed and calibrated.

Summary

Simplification and its ranking with regard to increasing levels of complexity have been discussed for several systems and unit operations, including:

- *Reactors*, using homogeneous gas and liquid systems, and heterogeneous systems (L/L, G/S and L/S, G/L , G/L/S). Although different systems have different simple designs, some overall conclusions can be drawn:
  - Adiabatic designs are favorable, and can be enforced on the system in different ways; these include higher reactant or diluent (solvent) flow, lower inlet temperature, and cold feed injection.
  - Non-adiabatic designs have an energy household which is preferably based on evaporative cooling followed by indirect heat transfer.
  - Heterogeneous systems are often limited by mass transfer; in such cases agitated stirred tanks are a poor choice. (Most developments on intensification concentrate on improvements on mass transfer limited systems; see Section 5.5.2.)
  - Multi-stage reactor systems and tubular reactors have a higher level of complexity.
- *Distillation* trains can be significantly reduced in the number of columns, by taking maximum benefit of dephlegmators, the application of side draws, and divided wall columns.
- *Extraction* operations are more frequently practiced as a multi-stage separation, which provides the opportunity to combine more extraction/wash functions within the same apparatus. Other advantages of multi-stage separations include increased extraction efficiency, with less solvent recovery. Thus, different types of columns are applied, from packed column, tray columns and mechanically agitated columns up to centrifugal extraction
- *Adsorption* is most commonly performed in fixed beds; indeed, the application of PSA at high-frequency switching for the gas adsorption desorption cycle is being increasingly utilized as a first choice.
- *Heat transfer* units are moving towards plate (finned) exchangers, next to the conventional types. This trend is based largely on the compactness and cost effectiveness of the plate systems.
- *Fluid transport* requires further emphasis on the application of gravity flow or pressure differences as driving forces. In this respect, the elimination of pumps and compressors should be the primary target.
- *Piping* may be a major contributor to complexity, and several guidelines have been developed to make piping systems more robust, and less complex.
- *Instruments* are the eyes, ears and hands of the process. The requirements on instruments concentrate on the robustness of the installed measurement. The avoidance of superfluous instruments is an option that is exploited by companies with remotely operated process in order to avoid call-out visits by engineers.

5.8 Contradiction between Simplification and Integrated Designs?

The consideration of whether combining functions into a single unit is in fact a contradiction of the term "simplification", has been the focal point of debate on more than one occasion. However, there are two elements which might be added to this argument and help to solve this apparent contradiction:

1. Understanding of the characteristics of the unit.
2. Are the number of DOFs for operation really increasing?

Nobody would argue against a need to *understand the characteristics of a unit* in terms of its operation, but to put this into perspective it may help to examine some well-known units and focus on their problem areas.

Although a pump – as every operator knows – can fail as a result of cavitation and dead heading, it is not always realized that the pump's characteristics are influenced by variations in its speed of operation. Likewise, for an adsorption unit, it is known that there is an adsorption isotherm applicable to the specific components to be removed, and that this is dependent upon the components" concentration(s). So, does the operator realize the consequences when the inlet concentration falls to a much lower concentration! And will a new equilibrium situation develop in the bed, perhaps resulting in a spontaneous breakthrough?

Our global understanding of a distillation column may be more obvious, but is it always realized that a temperature deviation occurring in the column might be caused by the introduction of components in the feed, and which might accumulate in the column? Initially, such an effect is not visible because the temperature is often not pressure corrected. Usually, the temperature is likely to be controlled, and so the column must first go off-specification before a problem is noticed. These are just some examples of problems that might occur among well-known unit operations.

For new unit operations, it is essential that the operation is fully understood, especially when there have been deviations from stationary conditions. The only effective way to achieve this is through dynamic simulation of the unit. Simple and robust process plants must be fully understood in order to permit automation, hands-off control, and adequate operational supervision. The modeling accuracy is not essential, although simplified reaction kinetics are often a requirement for this purpose, as long as all trends are representative of the operation.

If we examine reverse-flow reactors for catalytic combustion, the frequency of the reverse-flow actions has an effect on the reactor's performance, so must be understood. In addition, when the inlet concentration falls or rises, the reactor may either starve or over-heat – conditions which, again, require close examination and understanding. Although the design must accommodate for these situations, the operator must be aware of these potential problems and know how to react to their occurrence.

The same applies for units such as reactive distillation or divided wall columns. Gone are the days when the operator's experience of a unit was built up "on the job"- that is, when the process was itself in operation. Today, it is vital that we have a thorough understanding of a unit before start-up, and this knowledge needs to be used in the design of the automation, the control software, and for operation support. New designs are often not more complicated, neither are "Higee" devices especially complex, and only need to be understood in their specific situation.

A second point for debate is whether, in integrated design, the number of DOFs for operation are really increasing. For most integrated units, the DOFs are less than the summation of the separate units. In addition, the complexity factor (as defined in Section 2.2 in **Chapter 2**) is less for an integrated unit compared with summation for the separate units.

If we consider the reverse-flow reactor, a separate reactor with its heat train would certainly have a complex heat exchanger network in order to obey plug flow. It would also require similar provisions for starving the reactor, or to protect against its overheating. However, examination of a standard heat exchanger network with its control functions for such a system would increase the DOFs to some extent. A reactive distillation and a divided wall column also has fewer DOFs and a lower complexity than the sum of the separate units.

What will differ is the design of the control configuration. Knowledge concerning the unit, as captured in dynamic models, needs to be used to design a robust control configuration.

Unfortunately, the above do not always lead initially to simplicity. When we reexamine the design of the tubular reactor for oxidation (Figure 5.26), it becomes clear that the introduction of more injection points adds both to the DOFs and to the complexity. It should be recalled from the complexity term that this can be impacted by automation. The increased complexity of the reactor system had to be compensated for by improved control (Turunen et al., 1999).

Summary

The question of there is a contradiction between simplification and further integration of units can be discussed from two different viewpoints:

Understanding of the units is, and will always be, essential for adequate operation. From this perspective there is no great difference between new and older techniques, and each unit has its specific characteristics which need to be understood. The difference is that new designs must be initiated and operated based on knowledge – failure is no longer acceptable. In the past, older unit operations were often started and operated based on learning experiences, not today the only way to gain sufficient operational insight of a unit is through dynamic simulation. The modeling for this purpose does not require a high level of accuracy, but it does need to include simplified reaction kinetics.

The number of operational DOFs for integrated units is not, in general, increasing with respect to nonintegrated units. Indeed, most applications now show a reduction both in DOFs and complexity of operation. Some applications show an increase in those situations, an increased level of automation, and control in these cases is the requirement to cope with simple and robust process operational requirements. The higher level of automation and control must be supported by dynamic simulations and control design.

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Chapter 6
Process Design Based on Reliability

6.1
Introduction

Reliability engineering and probabilistic risk assessment represent a discipline which is becoming increasingly important in process design and operation in process plants. It is not only the design philosophy statement,

> *Design for single reliable and robust components unless, justified economically or safety wise*

that demands reliability engineering techniques and a probabilistic assessment. In an overview of the field of process design, operation and maintenance, it is possible to identify the areas where these techniques are mostly applied, including the following:

1. Evaluate a process design on availability and reliability based on mechanical failures rates of process equipment
2. Determine the optimal storage of feed and products based on the probability of raw material supplies, product delivery requirements, and processing reliability.
3. Evaluate the design of a chemical complex on its vulnerability resulting in product availability against mechanical failures for different levels of redundancy.
4. Evaluate process safeguarding systems, in particular instrumental protection systems, on the probability of failure on demand and nuisance trips.
5. Develop a predictive maintenance program based on failure rates.
6. Evaluate optimal spare part stocks.
7. Evaluate the probability of an incident of a process plant through quantified event and fault tree analysis.

The impact of reliability engineering is considerable, because many of the qualitative design guidelines that are currently in use – and often are quite conservative – can now be converted in quantitative approaches.

Reliability calculations can now support design decisions based on economics, while in the past these were based on arbitrary design guidelines. All decisions regarding the redundancy of equipment and other additional provisions can now be evaluated based on the difference in up-time of a process (operational benefits) versus additional capital investment. In this respect:

- Is there any value in the installation of a spare power supply cable to a process?
- Does the value of more up-time outperform the higher investment of the cable and its adjacent provisions?

Safeguarding of the process can now be quantified and the design protection level can be verified whether the required safety integrity level criteria are met, or not. In the past, design philosophies were applied as the levels of defense installed.

Maintenance departments found a valuable tool in reliability engineering to predict the failure of components that were subject to aging. A careful analysis of failure rates based on life data are used from the so-called Weibull analysis, in order to apply predictive replacement or repairs. The optimal amount of spare parts can also be determined, based on the failure rates of the components installed.

The basis for any quantitative risk analysis is the likelihood of an event (a failure) occurring, and this will be quantified, based on reliability data (CCPS, 1989).

From the above-mentioned application areas, only the first four have a direct impact on process design, and are described herein. In this chapter, the basic principles of reliability engineering are discussed. The evaluation of process design alternatives based on cost–benefit analysis will also be discussed in this chapter. The specification of design items which have an impact on process reliability and availability must be completed with a Reliability, Availability and Maintainability (RAM) specification. The reliability and availability requirements need also to be part of the contracts with suppliers, receivers and transportation companies, in order to enable an optimal reliable design.

The evaluation of optimal storage and the vulnerability of a chemical complex will be discussed in **Chapter 7**, safeguarding of the system being part of the instrumentation.

6.1.1
Reliability Engineering is an Evolution to More Optimal Designs

It must be said that reliability engineering techniques provide a support for economic plant designs. However, high reliability can only be achieved by good engineering practices. These practices are reflected in a reliability cycle (Figure 6.1), which shows a chain of activities that reflect the evolution of a reliable design. When we start at the top of the cycle, the process design takes advantage of databases to achieve an optimal design. This will include a RAM specification, if applicable. The design is translated by design engineering in selected equipment. After construction, the process will be taken in operation, after which maintenance becomes the first line involved in any repair ("Do maintenance"). The failure data are also col-

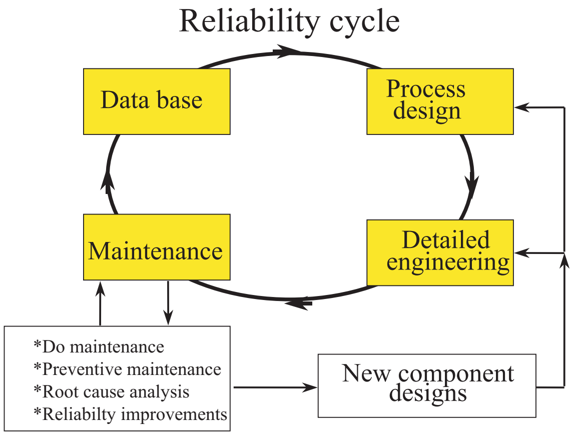


Fig. 6. 1. Reliability cycle.

lected and stored in a database, so that they are available for new designs. Next to a repair responsibility, the maintenance engineers also have as an objective preventive maintenance. From that perspective, they apply root cause analysis with production, and make proposals for improvements. After implementation of these modifications the engineers monitor specifically the mechanical performance of the process. Vendors are also approached to communicate performance data, and challenged to develop more reliable designs. Any improved designs must be implemented in new applications after thorough testing. All these activities are part of the ongoing reliability cycle (Figure 6.1).

The objective of this chapter is to make engineers aware of reliability principles and its application for process design. It should be noted that the process industry is not at the forefront in the application of this technology, but public power and distribution companies have been applying these techniques for many years. This was mainly caused by the drive for high availability and reliability requested by customers. Currently, reliability engineering techniques are used by the power companies to design reliable operation and distribution networks based on economies that are enforced by their competitive position. Electrical distribution systems require high investments in cables, transformers, switching stations with back-up provisions, and alternative designs are worth evaluating. The situation is similar to that of today's two-engine airplane which now operates as reliably as its four-engine counterpart of some years ago. The electrical industry invested in reliable and robust components to achieve a high level of reliability and availability. A similar pathway is followed by the computer industry, which must accommodate the requirements of their customers. Computer systems and networks (including system software) are subject to reliability analysis to provide very high levels of availability during working hours, while planned outages at off hours are still acceptable, but for how long? Nobody wants the network to be down, even at "off" hours, so that they sit in front of their screen, unable to work. The user software industry is lacking behind in that respect, but it will certainly need to comply with the market demands, or it will go out of business. However, user software is judged more on its on functional performance and robustness rather than its reliability.

The nuclear power industry was the first to use reliability engineering techniques on a large scale for the design of plants. However, it should be noted that this industry is still using many design conventions such as triple redundancy for instrumentation and the safeguard of equipment. Initially, some process and control designers were in favor of triple redundancy for process plants, but the battle has now turned in the delivery of safe plants complying with safety reliability criteria, as specified by IEC 61508. This opens the way for reliable instrumentation and safeguarding designs based on reliable and robust components in order to meet the criteria defined. A parallel can again be drawn with the two-engine airplane flying reliably and cost-effectively over the ocean!

The application of reliability engineering is the driving force in the development of an optimized design between suppliers and users of equipment and supplies. These optimal supplies can only be achieved in good partnership between supplier and user based on reliability data. This requires clever solutions to maximize reliability and availability at low cost (which is an evolutionary pathway), and not by extensive redundancy provisions. An over-demand from the user's perspective will result in more investment at the supplier, and this will ultimately result in higher product prices.

6.2 Basic Theory of Reliability

In this section, the intention is to introduce the most important terms as used in reliability engineering (Henley and Kumamoto, 1981 and 1992; Leitch, 1995; Red book, 1997), rather than to provide the reader with derivatives for these equations. However, this text is presented for use as a reference source for the methodology presented herein. In other words, how to apply reliability engineering to process design.

Reliability R(t) is defined a the probability that a component or system performs its function over a time interval 0–t (in a particular environment), given that the component or system was to be considered new at time zero.

Some definitions include the restriction "in a particular environment". The characteristics terms of the definition are:

- function
- time
- probability
- environment

The term *function* may appear simple in the case of a catastrophic failure, where it is easy to determine. A switch no longer works, so an electric device (e.g. a pump) cannot be started or stopped. In case of a drift failure, the function might undermine the performance and result in a catastrophic failure if no action is taken. An example is a vibrating pump which should be repaired before its ultimate failure.

The *time duration* – also called *mission time* – is a dominating factor. For a process plant this is the time between turn-arounds, and must not be confused with process stops for regeneration or cleaning. The time is an important aspect, as the reliability of components generally decreases with time. The reduction in reliability might also be affected by usage rather than time; for example, in the case of switches this would be the total number of times that they are operated, or in the case of a car, the mileage covered. In general, time is used as bases for comparison of reliability in the process industry, although it might be possible also to differentiate for specific units. For particular items that are subject to predictive/preventive maintenance (e.g. high-voltage power switches), repair regimes are often developed based on usage.

The *environment* will also have an impact on reliability; for example, an electric driver exposed to high temperature and corrosive atmosphere might fail earlier. The limitations are the number of data points available to determine the failure rates to a significant level. Due to this constraint, the environment is often broader than might be preferred.

Probability is the likelihood of occurrence of an event or a sequence of events during an interval of time, or the likelihood of success or failure of an event on test or on demand. Probability is expressed between zero and unity.

Reliability can be presented as a function of time in a history diagram (Figure 6.2). In such a diagram, the number of failures n_i, or the proportion of failures f_i, over a time interval t_{i-1} and t_i are plotted against time.

$$f_i = n_i / N$$

where N is the total number of items, and f_i is defined as the proportion of items failed between times t_{i-1} and t_i.

Fig. 6.2. History diagram of proportional failures against time.

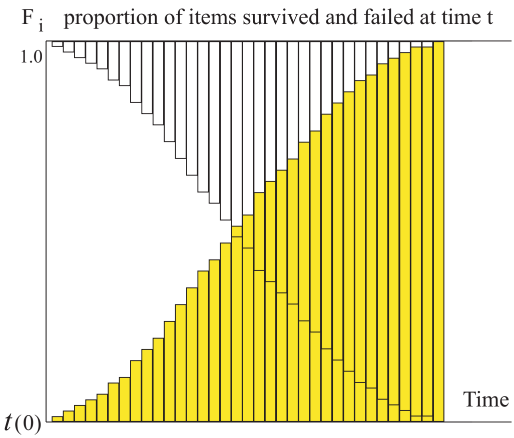


Fig. 6.3. Cumulative diagram of the probability of survival –F(t) and of mortality F(t) of components against time.

The same data might be plotted in a cumulative graph of F_i against time (Figure 6.3):

where $F_i = \sum_{j=1}^{i} f_j$,

and F_i is the proportion of items that fail by time t_i. It is clear that F_i increases with time and finally becomes 1.

Unreliability F(t) is defined as the probability that a component or system fails during the time interval (0, t) given that the component or system was to be considered new at time zero.

Reliability is the proportion of items that still functions by time t_i, which is equal to:

$$R_i = 1 - F_i \tag{1}$$

This relationship shows that R_i becomes 0 when $F_i = 1$, and the reliability R_i decreases with time opposed to F_i.

The *times between failures* are often used as, they express in a single number the result of a complex mathematical calculation. These may be defined as:

- **Mean time between failures** (MTBF) is the mean value of time length between two consecutive failures over a defined period (applicable for repairable items).
- **Mean time to failure** (MTTF) is the mean time of a component or system failure from t = 0 (applicable for nonrepairable items).

In formulae form, MTTF and MTBF for repairable systems are $= \int_0^\infty t\, f(t)dt$

- **Mean time to repair** (MTTR) is the time needed to repair a component; it includes not only the repair time but also includes the arrival time of the repair team and the spare parts. The component that failed also needs to be made available for maintenance and, after repair, the time monitored to put the component/unit/plant back in operation.

Now the failure rate is defined as:

$$\lambda_i = \frac{\mathbf{f_i}}{\mathbf{R_{i-1}}} \tag{2}$$

Failure rate λ(t) is the probability that a component or system, that survived up to time t, will fail in the next time interval.

When the failure rate of components is plotted against time, the graph often has the form of a bathtub (Figure 6.4). The initial zone A, representing the early failures, commences with rather high values, but these fall rapidly with time. At a certain moment the curve becomes relatively low and flat (zone B), and this represents a relatively constant failure rate. After a certain time, the failure rate increases again (zone C), which indicates wearing out (also known as "aging") failures.

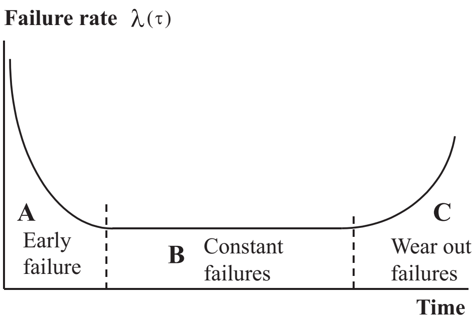


Fig. 6.4. The failure rate against time (the bathtub curve).

The early failures in zone A, which are relatively high, can be subdivided into the following categories:

- Design of the component
- Selection of the component
- Fabrication error of the component
- Installation error of the component
- Instrumentation errors of surrounding equipment, nor necessarily being a part of the component
- Operation mistakes, manual or automatic.

These potential errors are the main reasons why process plant start-up(s) deal with frequent starts and stops before being operated at a constant production level. Plant restarts suffer much less (even after an overhaul) when the number of new components is much less, although repaired devices might also fail due to maintenance errors.

The constant failure rate zone B represents the situation during the normal operational period of a process – the mission time. It should be noted that selection of the component is normally based on the low constant failure rates. The stand time of the components, before an increase in failure rates due to wear-out is noticed, should preferably exceed the mission time of the process. This does not mean there is no wear-out – only that there is no significant increase in failure rates due to wear-out.

The wear-out failures zone C represents a zone which is certainly entered by several components in process plants. Differentiation might be made between components here: (i) those which have very long life times (over 4–10 times the mission times, or 10 to 20 years), for example power cabling, windings of electric drives, lines or process vessels; and (ii) components which have a relative short lifetimes, for example 1.5–2 times the mission times. Both types are subject to inspections. The components with short lifetimes will be subject to repair during an overhaul in order for them to be considered as new. Consideration might be made to replace the bearings or seals of machines, or to replace frequently used switches.

The components with long lifetimes will be subject to inspection during overhauls or during operation, for example wall thickness measurements. A set of similar components which is under suspicion of wear-out failure can be identified using the Weibull analysis of life data (see referred literature). The identification of potential failures might be used for a maintenance plan to avoid unplanned stops.

6.2.1 Availability and Unavailability

Availability *$(A(t))$ is the fraction of time over a defined period (the mission time) that a component or system is fully operational.*

For a process plant, the mission time is the period between two overhauls (also called turn-arounds), and must not be confused with the time between planned process stops for regeneration or cleaning.

A time line is shown of a process in Figure 6.5, where the turn around is shown as well as planned stops for regeneration and stops for unplanned failures. The **maximum time available** is now the mission time minus time for planned process stops. The steady-state value of availability A is formulated as:

$$A = \left(\frac{MTBF}{MTBF+MTTR}\right) \tag{3}$$

A model for failure often applied is the constant failure rate, which corresponds to the zone B of the bathtub representation. The constant rate model is mathematically expressed as:

$$R(t) = e^{-\lambda t}$$

In this particular case

$$\lambda = \frac{1}{MTBF}$$

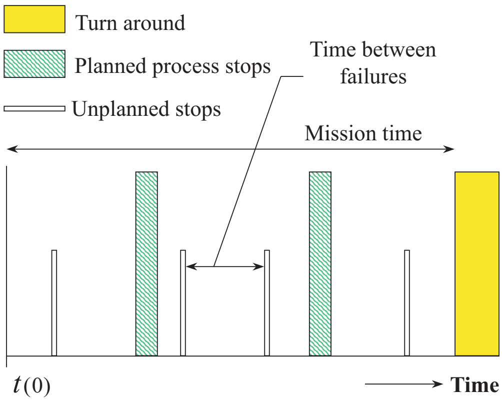


Fig. 6.5. Time line for a process plant.

With the constant failure rate, the relationship can be rewritten as:

$$R(t) = \exp\left[-\frac{t}{MTBF}\right]$$

Unavailability U(t) is defined as:

$$U(t) = 1 - A(t) \tag{4}$$

The unavailability due to failures (excluding regeneration stops) is expressed on a Markov technique.

When we write the mean time to repair MTTR as; $\theta = \dfrac{1}{\mu}$

$$U(t) = \frac{\lambda}{\lambda+\mu\left(1-\varepsilon^{-(\lambda+\mu)t}\right)} \tag{5}$$

derived by Markov analysis (Red book, 1997).

The limiting value average unavailability becomes: $\mathbf{U} = \dfrac{\lambda}{\lambda+\mu}$

The formulae can be simplified:

If $\mu >> \lambda$ and $t \geq \dfrac{3}{\mu}$ then $U(t) = \approx \dfrac{\lambda}{\mu}$

Or $\theta << \mathbf{MTTF}$ and $t \geq 3\theta$ then $U(t) = \lambda\,\theta$

As A(t) = 1 – U(t), the availability is now known.

The number of failures is $N(0,t) = \int_0^t \omega(t)dt$

where ω is the failure occurrence rate, which is the probability that a component fails during the next time interval, given that no failure will occur at time zero.

The failure rate occurrence becomes equal to the failure rate when we ignore the repair time as being small compared to the mean time between failures, then $\omega = \lambda$

Now, the number of failures becomes; $N(0,t) = \int_0^t \omega(t)dt = \lambda\, t$ (6)

6.2.2
Reliability Data and Distribution

Reliability data bases are available in the public domain for all kinds of components (CCPS, 1989; Oreda,1992). These databases embody not only the raw data but also the distribution functions with its parameters. Many larger companies have developed their own databases, but these are sometimes available for public data banks. The importance of a company's own database is that these can be made much more specific, especially with regard to the environment and the type of component. This can be helpful for the maintenance department, and also for the reliability engineer who will receive more specific information for new designs. The drawback is that the databank must be maintained for quite some time before sufficient data are available to obtain statistically relevant information.

Probability distributions We will now discuss some statistics relating to observations on failing components (events) as being the subject of reliability engineering.

*The probability (**P**) of an event is defined by Leitch as: "... the proportion of time that we observe that event in a large number of trials, or the proportion of time we would expect to observe, were we able to observe a large number of trials".*

Probability is also defined as: "... the likelihood of occurrence of an event (failure) or a sequence of events (failures) under stated conditions during a period".

Probability can be expressed as a percentage of failures, or successes, of the total number of trials; thus, the value will lie between 0 and 1.

There are, statistically, two important aspects relating to component or system failures:

1. The **average** or **mean value** (with its standard deviation).
2. The **mode of distribution**.

The average value (μ) for a discrete distribution is defined as:

$$\mu = \sum_{i=1}^{n} \frac{x_i}{n}$$

where n is the number of items, and x is random variable.

The average or mean value for a continuous function is:

$$\mu = \int_{-\infty}^{+\infty} x\, f(x)\, dx$$

The standardized statistical method to define the spread is through the variance, Var(x). For discrete distributions the variance is:

$$\mathrm{Var(x)} = \frac{\sum_{i=1}^{n} (x_i - \mu)^2}{n}$$

For continuous distributions, the variance is defined by:

$$\sigma^2 = \int_{-\infty}^{+\infty} (x-\mu)^2 \, f(x) \, dx$$

where sigma (σ) is the standard deviation.

There are different distributions that might describe the failure of components in time or any other usage function, though which distribution fits the best is a matter of evaluation. The different mathematical distributions are outlined in the following section.

6.2.2.1 The binomial distribution

This is commonly used to quantify the probability of failures for redundant installed systems. It is used to calculate the probability of failure on demand particular for safeguarding systems.

For k out of n systems, the system will fail if k or more components fail. The total failure probability is described by the cumulative binomial distribution.

$$\text{P (minimal k occurrences out of n trials)} = \sum_{s=k}^{n} \frac{n!}{s!(n-s)!} p^s (1-p)^{n-s}$$

where p is the probability of a system.

The mean is: $\mu = n\,p$, and the variance $\mathrm{Var}(x) = n\,p\,(1 - p)$.

The binomial distribution has only integer numbers for occurrences.

6.2.2.2 The Poisson distribution

This distribution is used when the likelihood of an incident occurring in the near future in not dependent on the occurrence or nonoccurrence of such an incident in the past. This can be the case when a process is producing components some of which do not pass the quality test (fail), and nothing is modified or changed on the process.

The Poisson function is defined as:

$$\mathrm{P(x)} = \frac{(np)^x}{x!} \exp(-np)$$

where x is the number of occurrences of a rare event ($p \to 0$). The Poisson distribution is a discrete probability distribution.

The mean value is: $\mu = n\,p$, and the variance $\mathrm{Var(x)} = n\,p$.

The Poisson distribution gives the probability of exactly x occurrences of a rare event with a large number of trials ($n \to \infty$); it approximates the binomial distribution when n is large and p is small. In other words, it describes the behavior of many rare event occurrences.

6.2.2.3 The exponential distribution

This distribution is frequently applicable to repairable systems, and is frequently used in reliability and safety studies. It implies that the failure rates are constant and independent, and so the mean time between consecutive failures is constant. Thus, the MTTF is equal to the MTBF. To illustrate this, when the bearings of a mechanical device fail and are repaired, the mean time to the next failure remains the same.

The exponential expression is $R(t) = e^{-\lambda . t}$ or $F(t) = 1 - R(t) = 1 - e^{-\lambda . t}$,

where λ is a constant failure rate.

Then, the expected number of failures in operating time period t is λ t.

6.2.2.4 The normal distribution

The normal distribution is in relation to a stochastic variable which can have values between ∞ and $-\infty$. The probability density function is:

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{t-\mu}{\sigma}\right)^2\right] - \infty < t < \infty$$

where the variable is t,

The mean value is μ, and the variance $Var(t) = \sigma^2$.

6.2.2.5 The log normal distribution

This distribution is often applicable to reliability studies. The variable t is said to be log normal distributed if ln(t) is normally distributed. The probability density function is now

$$f(t) = \frac{1}{t\sigma\sqrt{2\pi}} \exp\left[-\frac{(\ln(t)-\mu)^2}{2\sigma^2}\right]$$

$$x_{mean} = \exp\left(\mu + 0.5\sigma^2\right) \quad Var(t) = \exp\left(2\mu + \sigma^2\right)\left\{\exp\left(\sigma^2\right) - 1\right\}$$

6.2.2.6 The Weibull distribution

The Weibull distribution has a specific characteristic in that the distribution does not have a specific shape, but can have different shapes depending on the selection of a set of parameters. The distribution is commonly used in reliability analysis as it can describe decreasing, as well as increasing, failure rates. Earlier, we referred to the aging of components that are often covered in Weibull distributions.

The Weibull distribution for two parameters is defined as:

$$F(t) = \frac{\beta}{\eta}\left[\frac{t}{\eta}\right]^{\beta-1} \exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right], \quad 0 \le t < \infty$$

Where β is called the shape parameter (dimensionless), and η is called the scale parameter (dimension t). Increasing and decreasing failure rates are realized by the choice of the shape parameter β, where:

- β <1 indicates a decreasing failure rate;
- $\beta = 1$ indicates a constant failure rate; and
- β >1 indicates an increasing failure rate

There are more distributions, for example the uniform distribution, gamma distribution, and chi distribution. The most frequently used of these distributions have been mathematically expressed.

6.2.3
Estimation of Failure Parameters

The estimation of failure parameters is an important aspect of reliability engineering. The most advanced and accurate technique is based on large sample numbers, more than 30. The first step is to determine the type of distribution which best fits the data. For the different distributions under evaluation, the parameters are estimated to obtain an optimized fit of the data and the distribution function. How successful is the estimate can be expressed in the confidence interval of the final result. The distribution function is selected which best fits the data within the objected confidence interval limits. When these distributions and their parameters have been selected, the failure parameter can be derived directly from the distribution equation. The advantage of this approach is that the equations can be used as bases for the probabilistic models in Monte Carlo simulations, which solve large reliability problems, for example process designs numerical.

When smaller data sets are available (<30), other approaches such as the mean rank or median rank method are used. It must be clear that the smaller the data set, the more uncertainty there is in the accuracy of the data. This is presented qualitatively in Figure 6.6, where a plot is made of the inaccuracy in % against the number of failure showing the lines for different confidence levels as parameter. A quantitative diagram is shown in (Figure 4.8 of the "Red book" 1997) based on a chi-square distribution.

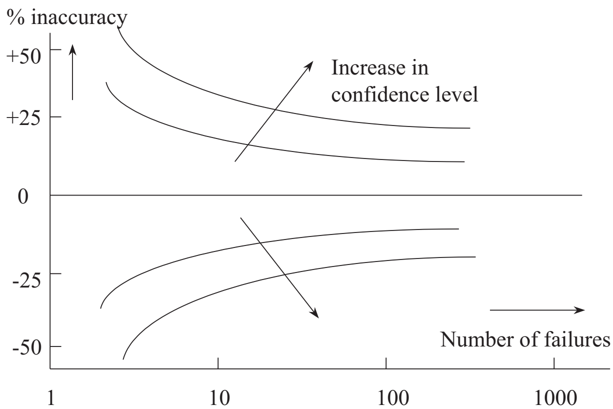


Fig. 6.6. The inaccuracy in % as a function of number of failures, qualitatively represented.

The different mathematical techniques for distribution analysis and the determination of the confidence are discussed in the referred text books. The selection of distribution models and its parameters is supported by commercial software packages, such as SPAR (Clockwork Design Inc.).

6.2.4
Reliability Modeling

Reliability block diagrams (RBDs) are used to develop models of a combination of components to complete systems (e.g. a process plant), and to calculate its reliability and availability performance.

A RBD is a simple model of a system which is represented as a pictorial representation of a reliability structure of a system (read in the context of this book, instrumental protection system, process unit or process plant). The diagram consist of a series of components or set of components represented as a chain. When one of the components (links) fails, the system fails.

If *redundancy* is build into the system, then it is shown as parallel components. So, for an application of a process plant, the RBD shows series and parallel components in a chain (Figure 6.7). Normally, the components are shown in order of processing, although for the calculation methodology this is not essential. In the example, one can represent each individual component or a set of components, such as a compressor or a gas turbine, or power generators. A set of components is used when reliability data are available for the set of components, mostly including its instrumentation. In other cases it is necessary to break the process down into its individual components. Supplies such as utility streams can also be represented as components.

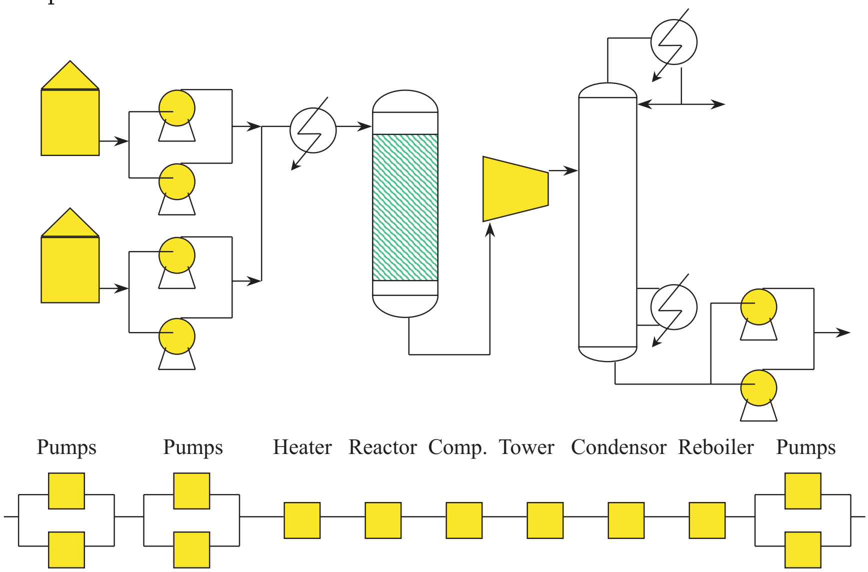
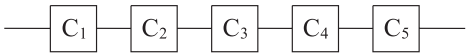


Fig. 6.7. Reliability block diagram for a process.

When only the process performance is of interest, the components of the supplies can be eliminated, or the reliability of the supplies can be designated as a one. All components in the RBD have their specific reliability data included in the model. The reliability model needs to have the capability of calculating the overall process reliability and availability, as well as identifying the individual, or groups of components, that contribute to the failure(s). The number of outages over the mission time are calculated, as well as the related down-times, and the contribution of the individual components are ranked. There are two techniques available for analyzing these problems: one is analytical, and the other is based on Monte Carlo simulations.

6.2.4.1 **The analytical technique**

The analytical technique is based on the *product and summation rules. The product or multiplication rule* is applicable when we have components in series whose failures are statistically independent. Such a system can only function if all components function.



The following mathematical nomenclature used is to define operations:

$\bigcup$ Operation of union

$\bigcap$ Operation of intersection

$\overline{C}$ Operation of complementation

In other words; $\overline{C}$ = Component C is down, C = Component C is up

The probability (P) that the system is up is the product of the probability each component is up. In formulae, this is expressed as:

$$\text{P (system is up)} = \text{P}(\text{C}_1)\ .\ \text{P}(\text{C}_2)\ .\ \text{P}(\text{C}_3)\ ....\text{P}(\text{C}_{\text{n}}) = \prod_{i=1}^{n} P(C_1) \tag{7}$$

The system will not perform the function or the system is down is described as:

$$\text{P (system is down)} = 1 - \text{P (system is up)} \tag{8}$$

This can be written in two ways:

$$\text{P (system is down)} = 1 - \prod_{i=1}^{n} P(C_1)$$

or

$$= 1 - \prod_{i=1}^{n} (1 - P(\overline{C_1})) \tag{9}$$

The possibility that two components fail at the same time is very low, when the probability of failure is $P(\overline{C}) < 0.1$.

In that case, the probability that the system is down is reduced to the following approximation:

$$\text{P (system is down)} \approx \sum_{i=1}^{n} P(\overline{C_1}) \tag{10}$$

This last reduction is called the *rare event approximation*.

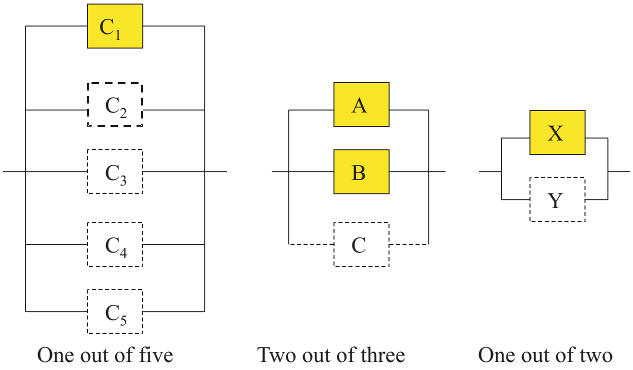


Fig. 6.8. Parallel components for different configurations.

The *summation rule* is applicable to systems with parallel components, and failures of these components are mutually exclusive. In a parallel system, the overall system fails if all the subsystems fail. A parallel system is shown in Figure 6.8 for different configurations: one out of five; or one out of two only fails if all parallel components fail. This is expressed mathematically as:

$$\begin{aligned} \text{P(system is down)} &= \text{P}\ (\text{C}_1 \text{ down} \bigcap C_2 \bigcap C_3 \ldots \bigcap C_n) \\ &= P\left(\overline{C_1}\right) \cdot P\left(\overline{C_2}\right) \cdot P\left(\overline{C_3}\right) \ldots P\left(\overline{C_n}\right) \\ &= \prod_{i=1}^{n} P\left(\overline{C}\right) \end{aligned} \tag{11}$$

For the system two out of three, Eq. (11) becomes:

$$\begin{aligned} \text{P(2/3 system fails)} &= \text{P}\left\{\left(\overline{A}\bigcap \overline{B}\right)\bigcup\left(\overline{A}\bigcap \overline{C}\right)\bigcup\left(\overline{B}\bigcap \overline{C}\right)\right\} \\ &= \text{P}\left(\overline{A}\bigcap \overline{B}\right) + \text{P}\left(\overline{A}\bigcap \overline{C}\right) + \text{P}\left(\overline{B}\bigcap \overline{C}\right) - 2.\text{P}\left(\overline{A}\bigcap \overline{B}\bigcap \overline{C}\right) \end{aligned} \tag{12}$$

The results of serial and parallel systems are tabulated in Table 6.1. The probability of failures for the different configurations have been calculated for two probabilities of component failure 0.1 and 0.05. The failures are assumed to be mutually exclusive. The configurations which have been calculated are:

- Serial components, one up to five with Eq. (7) and approximated with Eq. (8)
- Parallel components one up to five with Eq. (11)
- Parallel components two out of three with Eq. (12)

The results of the table clearly lead to the following conclusions:

1. Decrease in probability of component failures give higher system reliability
2. More components in series goes at the expense of system reliability
3. The approximation equation for serial systems is accurate for small failure probabilities and a limited number of components in series

Table 6.1. Probability of failures for serial and parallel systems for two probabilities of component failures 0.05 and 0.1, it is assumed that the failures are mutually exclusive.

System	*Probability of failure 0.05 Eq. (9)*	*Probability of failure 0.1 Eq. (9)*	*Probability of failure 0.05 Approx. Eq. (10)*	*Probability of failure 0.1 Approx. Eq. (10)*
Serial components				
1	0.05	0.1	0.05	0.1
2	0.0975	0.19	0.1	0.2
3	0.143	0.271	0.15	0.3
4	0.185	0.344	0.2	0.4
5	0.226	0.41	0.25	0.5
Parallel components	Eq. (11)	Eq. (11)		
2	0.0025	0.01		
3	0.000125	0.001		
4	0.0000062	0.0001		
5	0.0000003	0.00001		
	Eq. (12)	Eq. (12)		
2 out of 3	0.00725	0.028		

4. More parallel components leads to higher system reliability
5. The two-out-of-three systems have a system failure probability between a single-component system and a one-out-of-two component system. These systems are often selected as they are also used for error detection in case deviations between measurements are notified.

6.2.4.2 **Monte Carlo simulations (Dubi, 1998)**

Practical problems in reliability engineering cannot be, or are difficult to be, solved analytically. The reasons behind this are: the size of the problem becomes too large and the distribution functions of the input data are difficult to handle. Therefore, the analytical problem-solving techniques are limited to smaller problems where average values are used as input.

The best practice for large problems is to build a probabilistic model of the problem. The model is based on the RBD structure, while the input data are randomly selected from its probabilistic distributions by a random number generator, often called RAN. The random generator needs to be adapted to the distribution functions as applicable to the different components. The model is run in time for a large number of cases, each case with a new random selected set of input data. Each run provides a success or failure of the system model, and the cause of a failure. Based on the accumulated probabilistic results the reliability of the system with its distribution is calculated. Reliability programs are equipped with a clock to monitor the data over time. The type and number of failures over the mission time is recorded, as will be the related down-times. The down-times are converted in system availability. Such a Monte Carlo simulation can easily be adopted, which makes the evaluation of alternatives easy. This technique is used to evaluate all kinds of systems, and is not specific for process plants. A commercial reliability engineering tool (e.g. the software named SPAR, from Malchi Science Ltd., Israel and licensed by Clockwork Design Inc.), is equipped with a Monte Carlo simulator.

6.3 Methodology of Reliability Engineering Techniques for the Design of Process Plants

During the discussion of design philosophies, the starting point for the design was:

Design for single reliable and robust components unless, justified economically or safety wise

This means that the starting point for a design is as simple as possible, and that any deviation from this point needs to have a justification. At this point we will limit the discussion to an economic justification.

The *methodology* applied for reliable process design (Shor and Griffin, 1991; Koolen et al., 1999) is discussed step by step. The questions to be addressed, to achieve an optimal design regarding process reliability, relate to the reliability and availability for different process alternatives:

- Reliability – to be split into type and number of failures over mission time and its distribution.
- Availability over mission time minus its planned process stops based on any unplanned outages for failures categorized per component or set of similar components.

The methodology is addressing the mechanical reliability of the process, the process reliability being covered under planned process stops. The availability of feed and requirements on product availability are beyond this process design discussion, and these aspects are discussed in **Chapter 7** under storage optimization and site vulnerability.

The successive steps to be taken are:

- To set up a multi-disciplinary reliability team. The reason is that this is a rather young technique which requires input from different sides to obtain a good and acceptable result. The following disciplines need to be represented by: a production engineer, a maintenance engineer, reliability engineer, process engineer, and an economic evaluator. All their inputs are crucial for a sound, reliable process design.
- To develop a RBD from the primary flowsheet, which needs to visualize the reliability process. The RBD is based on the index flowsheet, and shows all serial and parallel equipment in a block diagram. The RBD includes blocks for utility supplies and any direct feeds. The streams from and to tanks are excluded, but this point will be discussed under design of storage facilities.
- To collect reliability data for all components or a set of components, including its distribution. This is a time-consuming effort, although most of the col-

lected data can be used for other designs. Sources are the public data banks (e.g. Oreda, 1992; CCPS, 1989). On occasion, we might receive data from equipment suppliers for complete systems such as compressor stations, gas-turbine systems, and power generators. Care must be taken not to use the supplier's guaranteed data as these are conservative, but an attempt should be made to obtain actual performance data. These are, in general, quite accurate. Collect the company reliability data, particular for components in a specific service and utility supplies. It may be useful to confirm the utility data with a detailed reliability study of the utility systems, complete with its redundancy and load shedding system (see **Chapter 7**). Some overall data for process equipment are shown in Table 6.2, though these are to be used for reference, and not for design.

- To collect repair and process interruption times, and to set mission time(s). Repair times must be determined per item, including the time required for spare parts to be available at location. Critical spare parts selected at its availability and failure rate might be available at the site. Repair times need to be supported by maintenance, as they have an impact on the organization, since maintenance people on call need time to arrive at the location. Process interruption times have to be determined with production per item. These times include the time required to make the failed component available for maintenance, and it also emphasizes the time required to get back into production. Repair times are not included. The repair and process interruption time together set the system unavailability per component per failure.
- Mission time has to be set. For continuous plants, mission times of 4–5 years have been shown to be achievable for world-scale plants. The mission time is set by:
- – Inspection time of specific items, such as pressure vessels.
- – Maintenance on components which become subject to wear-out, for example seals and bearings, and those subject to erosion and/or corrosion.
- – Process improvements to upgrade economically the plant, together with evolution of the technology.
- To quantify next to repair cost, any cost-related to process damage as a consequence of a failure. Any process damage might result in high cost as per: rework of product, additional production loss as a result of lost batches, equipment damage which is sometimes applicable to high-temperature processes or polymerization processes. These cost data are in addition to any lost production capacity due to unavailability of the process. These cost data are needed for the evaluation of project alternatives.
- The model has to run, to collect, and to accumulate the reliability and availability data. The probabilistic simulations must run for sufficient time to obtain statistically relevant information. The experienced gained for a process plant run time over 50 years and a random number of input data selection of 100 was sufficient, though this must be confirmed by making initially some more runs. The following data are collected over the mission time:

- Total number of outages.
- Outages per group of similar components or individual components such as pumps, vessels, compressors, and exchangers.
- Total lost time (unavailability).
- Lost time per group of components or individual components.
- Ranking items in order of failures/outages and time lost.

• Evaluation of results and development of alternatives. Evaluation of performance make the components that contribute mainly to failures and unavailability clearly visible. Also, the cost of these outages can be related to the different components. In line with the design philosophies for simple and robust process plants, we must evaluate the following options to meet the objectives:

- Can unreliable component be avoided? Examples to be considered include: replacement of a pump by taking advantage of gravity flow or pressure difference, or replacement of an agitator by a jet mixer.
- Consider replacement of less reliable components by more reliable ones. Examples include: replace liquid sealed pumps with seal-less pumps, or provide gas seals; alternatively, compressors might replace liquid seals by gas seals An agitator with a long shaft might be replaced with a bottom entry agitator. The long shaft of an agitator creates large forces on the bearings and seals, due to any imbalance of the rotor, and may be subject to extreme wear.
- Identify components as *less critical*.
  In some situations, as in the case of pump failure, these failures do not have to result in a momentary process stop. When a process can withstand this interruption during the MTTR of the pump, then it is called a "non-critical" item. This might be the case for some dosing pumps. For example, cooling water systems but also boiler water systems can stand interruption for several hours. In those cases, we can compensate the interruption by a temporarily higher dosing stream after repair.
  Another option to be explored is to build some temporary hold-up in the process. The bottom hold-up of a distillation tower might be increased to capture the volume of a small tar stream during a short outage of the bottom pump. The same applies to the size of a reflux drum in case of a small top product stream.
  Consider installation of redundant components. The redundancy of items should be the last explored option for a design, although there might be no other choice – particularly in the case of damage situation after a failure. The option of sharing an installed spare needs to be explored, for noncompetitive process streams, in terms of safety or product quality. One should respect total quality control (TQC) as objective.

Note: In the above, most attention has been paid to rotating equipment as being one of the major contributors to component failures. Much progress has been made during the past few decades on dynamic seals and bearing development, in order to make the design more robust.

Operation by automation easily respects the design conditions of the equipment, resulting in the avoidance of cavitation and deadheading of pumps, and surge or choking of compressors. Frequency analysis of signals from instruments installed close to rotating equipment can be applied to identify (alarm) any miss operation. The lifetimes of these devices can exceed current MTBF values by using these more robust operational practices. Another example is that of an agitator which must be always submerged in service and provided with a proper vortex protection and signal analysis warning to obtain longer stand time. The failures of rotating devices are mostly related to its miss usage and less to wear out.

Examples of highly reliable rotating equipment include steam turbines, electrical generators, and centrifugal compressors, for which the MTBFs exceed stand times of five years.

The above points of better design and improved operation by automation will still improve the failure rates.

- The evaluation and selection of the most economical alternative is the final step for the design. This is the trade-off between investment cost and production losses. The losses due to unplanned outages need to include any damage inflicted as a result of process interruptions.

Validation is an important aspect of reliability study. The basis for the study is formed by the failure rates and its distribution. An additional confirmation of the results is still a valuable exercise. The best way is to compare the overall results of the study by the evaluation of similar process plants during their history. The most striking results were obtained by comparing the results of a polypropylene reliability study with the data of an engineering company. This company licensed globally dozens of similar plants, and collected for years all failure data from these processes. The comparison that was made showed that the reliability and availability data had a very good fit with the study results.

6.4 Application of Reliability Studies for a Process and Utility Plant

6.4.1 Application of a Reliability Study for a Continuous Process Plant

The production of 1-octene from crude C4, is subject to a reliability study. Thus consists of three process sections, as presented in Figure 4.2 **Chapter 4** (Koolen et al., 1999). In the reliability study, we examine the mechanical reliability of the telomerization section. The connection between process sections through intermediate storage will be discussed with respect to availability in **Chapter 7.**

In this study, the utility failure rates were set at zero, while planned process stops for catalyst regeneration and fouling were not considered as unavailability. This gives a clear picture of the process itself.

A base case (case 0) was selected for the design with single components with an exception for those components which also served another process section. This was to avoid outage of more sections/plants by failure of a component. This approach is common to be followed in designs where independent operation of process sections/plants is the selected operational strategy. The results of the base case are given in Table 6.3.

It is clear from the data that pumps make the major contribution to mechanical failures, and the number of unplanned stops (6.4 per year) was considered quite large. The total number of pumps was 15, and the number of installed spare pumps was five. The average repair time for the pumps in this study was 12 ± 2 h.

Table 6.2. Overview of some typical MTBF, MTTR (h), and its distribution function of process equipment.

Component	*MTBF*	*Distribution*	*MTTR*	*Distribution*
Drum/vessel	920 000	Exp.	60	Exp.
Column	162 000	Weibull	120	Log N
Agitator	31 500	Weibull		Exp
Compressor	13 000	Exp	32	Log N
Pump liquor seals	9 900	Weibull	12	Log N
Pump gas seals*	19 800	Weibull	12	Log N
Seal-less pumps	12 600	Exp	12	Normal
Vacuum pump	13 500	Weibull	12	Log N
Exchanger	108 500	Log N	20	Log N
Condenser	107 700	Exp	20	Log N
Reboiler	150 000	Weibull	20	Log N
Air cooler	29 300	Weibull	12	Normal
Centrifuges	13 000	Exp		

* Limited data are available, but comparison between liquid and gas seals for compressors justified doubling of MTBF.
Note: Repair times of pumps are based on replacement of pump by spare pump at stock.

Table 6.3. Base case 0, overview of down-time and number of stops and unavailability as function of type of mechanical equipment failures.

Type of equipment	*Down-time (h/year)*	*No. of unplanned stops/year*	*Unavailability as % of time*
Pumps	61.9	5.1	
Heat exchangers	24.4	1.3	
Drums	7.7		
Columns	2.4		
Rest of equipment	1.9		
Total	98.3	6.4	1.12

Several alternatives were evaluated for different pump configurations, as these had the major contribution to down-times and the number of unplanned stops per year. The alternatives evaluated were:

- **Case 1:** the same as base case (0), but with four pumps identified as noncritical. Noncritical is defined as a situation where a process can stand a failure without interruption within the MTTR of the item and its distribution.
- **Case 2:** as Case 1, with two additional spares for those cases which had rather long process recovery times.
- **Case 3:** as Case 2, with pumps in which the MTBF was extended two-fold by the application of gas seals.
- **Case 4:** all pumps spared.

The results of the reliability calculations are listed in Table 6.4 for the contribution of pumps. It is clear from these results that single pumps provided with gas seals (Case 3) give a large reduction in down-time as well as in the number of unplanned stops per year, which clearly will have a positive economic outcome. The investment cost of gas seals is marginal compared with the savings in reliability and availability The spare pumps have the highest reliability and availability, but that is not necessarily the best choice. In most cases, investments in reliable components have a shorter payback than an increase in redundancy, this is already practiced for years in case of compressors.

Table 6.4. The contribution of pump reliability for several design cases on: down-time/year, number of stops/year, overall process unavailability, including all equipment.

Alternative	*Down-time (h/year)*	*No. of unplanned stops/year*	*Unavailability as % of time*
0	61.9	5.1	1.12
1	48.6	3.2	0.92
2	34.2	2.45	0.80
3	16.1	1.	0.57
4	0.	0.	0.42

The above illustrates that reliability engineering techniques can easily be used to design an optimal reliable process. In the next chapter, the reliability of a process will be studied in the context of a complex of integrated process plants including feed supply, product delivery, and utilities.

6.4.2 Application of a reliability study for a utility steam plant

Reliability engineering studies for utility plants are, in essence, not different from those for process plants, but the economic optimal levels of reliability and availability are much higher. Any outage on utilities – whether power, steam, process water, central cooling water system, fuel-gas, or instrument air – may lead to total site outages.

The cost of theses outages may be high. Site vulnerability is discussed in the next chapter. Here, the results of a study by Shor and Griffin (1991) are summarized, regarding the design of co-generation plants to provide a reliable, continuous steam supply.

The objective for the study was to evaluate the reliability of steam supply of minimum 380 Mton/h for different co-generation design cases. Four design cases were considered, while case 2 had a variant A and B (see Figures 6.9 and 6.10):

- **Case 1** consisted of three gas turbines (GT), frame 6, each provided with a waste heat boiler (WHB) and two existing fossil boilers (FB).
- **Case 2** consisted of four gas turbines LM 2500 with WHB and two existing fossil boilers.
- **Case 2** (A and B) differentiate themselves in the capacity of the WHB, 75 versus 100 Mton/h.
- **Case 3** consisted of three boilers with steam turbines provided with back-up de-superheaters and the two existing FBs.
- **Case 4** emphasized four large-capacity boilers with three steam turbines provided with de-superheaters.

The maximum steam and power capacities for these cases are summarized in Table 6.5. The steam production of these cases is also given if a boiler or a turbine is eventually combined with a WHB is out of service. In all these cases the minimum amount of steam (380 Mton/h) is still available. This is a design requirement, as utility plants have to provide their service all-year round, and so scheduled maintenance needs to be performed during operation. At a small site, the maintenance of utility systems might be performed during planned process plant stops. For the dif-

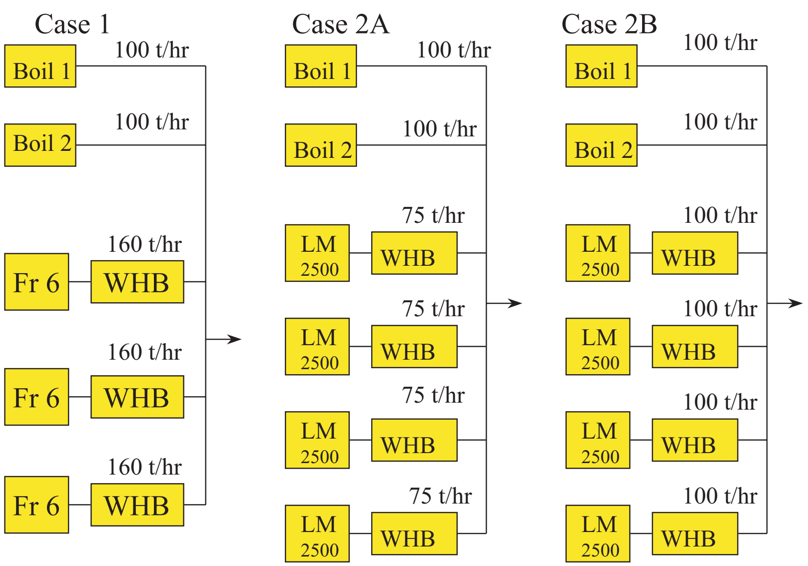


Fig. 6.9. Alternative designs for a co-generation plant.

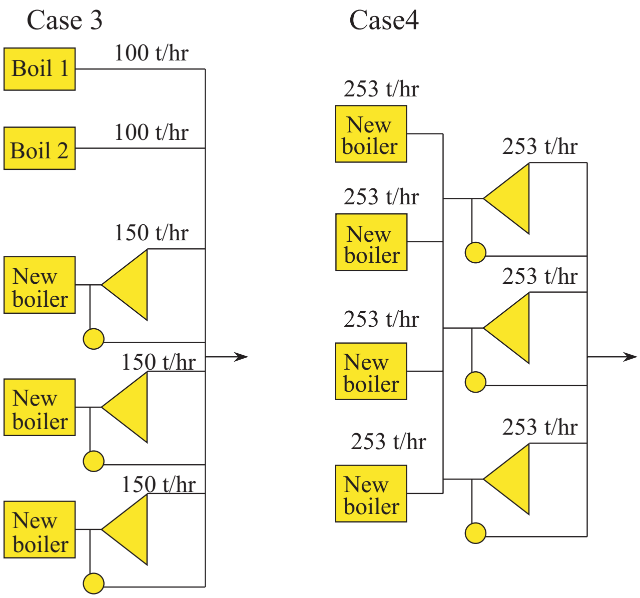


Fig. 6.10. Alternative designs of a co-generation plant.

ferent cases a forced outage during a scheduled maintenance stop of one of the units does not necessarily result in a shortage of steam.

The objective of the study was to quantify reliability of the steam supply for the different design cases. The reliability of the power supply was outwith the scope of the study, and it was assumed that a sufficiently sized external power supply was available as back-up.

The results of the study should be used as input for an economic evaluation to optimize investment in utility plant reliability versus cost of a temporary reduced steam supply. The cost of a reduced steam supply might be minimized by the application of an on-line steam load-shedding system, which has the advantage of avoiding total site outage by selectively shutting off steam consumers. These systems operate in the same way as power load-shedding systems.

Table 6.5. Full load steam capacity (Mton/h) for the different co-generation system cases.

Cases	*Max. MW*	*Max steam (Mton/h)*	*One boiler in shut down Max steam (Mton/h)*	*One turbine in shut down Max steam (Mton/h)*
Case 1	111	680	580	520
Case 2A	80	500	400	425
Case 2B	80	600	500	500
Case 3	111	650	550	500
Case 4	174	1010	760	1010

The reliability study is approached somewhat differently to that for a process plant. Utility plants are designed and operated to provide their an ongoing service, at a certain level. Therefore, the mission time is set at one year (not between turnarounds), while shutdowns for maintenance are scheduled over the year without interruption of the supply. These shutdowns – called scheduled outages – must be incorporated in the reliability approach.

The collection of reliability data is an essential step, and the failure data and scheduled outages and forced outage data are summarized in Table 6.6. The failure data of gas turbines includes the generator, WHB, and the feed supplies. The failure data for the boilers includes the steam letdown stations and feed water supplies. Steam turbine failure rates were not included as the system was provided with de-superheaters for bypass operation. The scheduled outages for the frame 6 gas turbines were explicitly higher than from LM 2500 turbines, as these require longer overhaul times.

Table 6.6. Data used for reliability calculations of co-generation plant.

Units	*Scheduled Outage factor (SOF)*	*Failures/h (MTBF in h)*	*EFOR Unavailability per year by forced outages*	*Equivalent availability factor (EAF)*
Fossil boiler	0.0301	0.000559 (1788)	0.0482	0.923
Gas turbine frame 6*	0.047	0.000978 (1022)	0.0448	0.91
Gas turbine LM2500*	0.029	0.000978 (1022)	0.0448	0.927

SOF (scheduled outage) is the proportion of calendar time that a unit is down for scheduled maintenance.
EFOR (equivalent forced outage rate) is the unavailability caused by forced outages in proportion of calendar time.
EAF (equivalent availability factor per year) is the availability of the unit per year including shutdowns and forced outages. EAF = (1 – EFOR) (1– SOF).
* Failure rates based on triplex control system.

It should be noted that the failure rates for these gas turbines are far too high for process application. The frame 3 GTs, as applied in process plants, are very robust, have a stand time of over 4 years, and are on the critical path of extending the time between turnaround. GTs for utilities plants (e.g. frame 6 and LM2500) are selected primarily for high efficiency, this at the expense of reliability and availability. The GT manufacturers must be challenged to improve the failure rates of these machines.

The assumptions made for this study were:

- Frame 6 failure data were based on a highly reliable triplex control system.
- LM 2500 failure data included simplex and triplex control system in the final calculations.
- The failure rates of the LM2500 GTs are not affected by a larger size WHB.

- The calculation method assumes that all the steam-producing units are operational, except when they are on scheduled or forced outage.
- Only one unit is scheduled for an outage at a time.
- Common mode failures are not assumed for the different units, including electrical power losses.
- Electrical power reductions are assumed not to have an effect on the steam generation.

The results of the reliability study are summarized in Table 6.7, the conclusions being that:

- Case 4 has the lowest failures per year, as the number of spare units is still one during a scheduled outage. The failure rate of a boiler unit is low compared with the systems with a GT, which have high failure rates.
- Case 2, being the lowest performer, is analyzed. It is clear that there are relatively cheap methods to decrease the number of forced outages. First, a triple redundant control system halves the number of forced outages. Second, an increase in the duty of the WHB with 33% reduces the number of failures per year from 11.7 to 1.6 for the triplex control system, a decrease by a factor 10. These actions would bring the performance to the next best.

Table 6.7. Number of failures per year to supply 380 Mton/year steam.

Cases	*Failures per year*	*Failures per year*
Case 1	4.2	
Case 2 A	23.4 (Simplex)	11.7 (Triplex)
Case 2 B	3.2 (Simplex)	1.6 (Triplex)
Case 3	2.1	
Case 4	0.22	

Overall conclusions of the reliability study of the utility system

- The results form a good basis for an economic evaluation to select the optimal utility system.
- The impact of process failures on a site might be reduced by the application of a steam load-shedding system. Such a system should be part of the evaluation, as it is relatively cheap to operate, and easy to implement with current control techniques.
- The results depend heavily on its assumptions, to mention specifically common cause failures. The design of each system should be totally independent to achieve the calculated failure numbers. The feed water system with its treatment, e.g., is commonly shared with other boilers, though this would require a specific reliability study. A detailed RBD and its quantification with all interacting components will show the weak points in the design. This is also applicable for other boiler-related systems which are shared. An error here might lead to total forced site outages, with associated very high cost penalty.

The reliability analysis was performed by the authors based on an analytical technique. The same calculations could be carried out using Monte Carlo simulations. In the last case, different types of failures and its distribution on failure and repair rates might have been introduced. The overall conclusions would not be any different, but especially the impact of more specifically identified components and their failure rates might provide a prioritized picture of causes of the failures and their impact.

The overall conclusions of the above application studies are that reliability engineering tools are very useful in the quantitative analysis and support of design decisions. The weak components with regard to reliability and availability are easily identified. Often, technical solutions can easily be found or developed to increase the reliability of these components.

6.5
Reliability, Availability and Maintainability (RAM) Specification

The purchase of equipment and supplies will, next to design specifications, at least partly be accompanied by RAM specifications. These cover the quality of the equipment in terms of reliability, availability, and maintainability. For supplies such as power steam (and also other supplies), the RAMs cover the reliability and availability of the supplies, as well as the reliability and availability of transportation of feed streams and product streams.

The RAM data require a partnership between the supplier and the receiver, and strong arguments exist for this statement:

1. The receiver is going to design and optimize his/her facility based on these data.
2. The supplier needs to optimize his/her facility on these data.
3. The data as such should be established in a realistic agreement as they represent a trade-off between the supplier and the receiver interest.
4. The agreed RAM data need to be realistic and supported by historic data.
5. An agreed measurement system must be established, especially as the data are subject to fluctuations and require a minimum number of data points over an extended time horizon. In this respect, a failure should be clearly defined at this point.

The RAM specification should consist of the following items:

- Scope of the system;
- – a description of the system
- – the life time
- – operating conditions
- – failure cases
- Quantitative requirements
- – availability
- – failure rate
- – time to repairs
- – scheduled outages

- record keeping of failures and repairs
- Perform a Failure Mode and Effect Analysis (FMEA)
- To achieve a good understanding of the system, a FMEA is performed, whether qualitative or quantitative. This provides a good insight into the operational/ automation procedures required, and identifies potential failures which are an input for the spare parts needed to cope with availability requirements.
- Maintainability has affects in three ways:
- the time to repair, and its impact on availability
- cumulative costs
- repair quality

The different issues need to be covered by both the vendor and user, and the responsibilities determined for each partner documented.

During the development of a RAM specification it should be realized that there is no “free ride”. A 100% reliability and availability does not exist, and a very high requirement is something that the user has to pay for. When we examine the power supply, everybody prefers 100% reliability and availability. Such a requirement will certainly be very expensive, as it would require high investment in redundancy for generation, back-up supply, transformers, cables, and switching stations. The level of reliability and availability is an overall optimum covering both user and supplier, while cost will always be the final product.

6.6 Summary

Currently, reliability engineering receives an increasing amount of attention in process design, the objective being to develop reliable yet simple and robust designs. This can be achieved by the application of reliability engineering techniques based on historic failure data, and the evolution to more robust equipment designs. The following points have been discussed in this chapter:

- The basic theory of reliability
- The development of reliability flowsheets (RBDs) and analytical and Monte Carlo solving techniques. Using these techniques, the reliability and availability of processes can be quantified based on the historic data of the components.
- The methodology for the development of an optimized design of a process plant.
- An application for a process plant, with process alternatives being compared in order to obtain an improved reliable design.
- An application of a utility plant, where several alternatives were compared.
- A good partnership between a vendor/supplier and the user is a primary requirement to develop and maintain a RAM specification for optimal process design.

6.7 Definitions

Availability A(t) is the fraction of time over a defined period (mission time) that a component or system is fully operational.
Common cause failure is the failure of more than one component or system due to the same cause.
Failure rate λ(t) is the probability that a component or system, which survived up to time t, will fail in the next time interval.

$$\lambda(t) = \frac{f_i}{R_{i-1}} \quad \text{and} \quad f_i \quad \text{is} \quad \frac{n_i}{N}$$

where; n_i is the number of items failed in the ith interval
N the total number of failed items over the test period
R_{i-1} is the reliability at time t_{i-1}
Failure occurrence rate ω(t) is the probability that a component or system fails in the next time interval not necessarily for the first time, with no failure at time zero.
Mean down-time (MDT) is the fraction of the mean time period observed that the system cannot perform its function. MDT is the MTTR plus the mean time to take the system out of operation for maintenance, plus the mean time to take the system back in operation.
Mean time between failures (MTBF) is the mean value of time length between two consecutive failures over a defined period (applicable for repairable items).
Mean time to failure (MTTF) is the mean time of a component or system failure from t = 0 (applicable for nonrepairable items)

In formulae form; $\text{MTTF} = \int_0^{\infty} t\, f(t)dt$

Mean time to repair (MTTR) is the mean time taken to repair a component. This starts at the moment a component is available for maintenance and continues until the time it is made available for operation to return to service. The repair time includes travel time, diagnosis, waiting time for repair items, and actual repair.
Mission time is the time between turnarounds, and should not be confused with the time between planned shutdowns for regeneration or cleaning; for continuous plants, this may be 4–5 years.
Probability (P) is the likelihood of occurrence of an event (failure) or a sequence of events (failures) under stated conditions during a period. The probability is expressed as between zero and unity.
Probability density distribution f(x)

The probability density function is $f(x) = \frac{dF(x)}{dx}$

Probability distribution F(x) The probability distribution of a stochastic variable x means the set of all values of x with the related probabilities
Probability of failure on demand (PFD(t)) The probability of failure on demand is the likely hood a systems is down at time t and unable to operate if requested.

Reliability R(t) is the probability that a component or system performs its function over a time interval 0–t, given that the component or system was to be considered new at time zero.

Unavailability U(t) is defined as U(t) = 1 – A(t)

Unreliability F(t) is the probability that a component or system fails during the time interval (0, t) given that the component or system was to be considered new at time zero:

$$F(t) = 1 - R(t)$$

Notation

A(t)	availability
f(t)	proportion of items failed in time interval
F(t)	unreliability
n	the number of items or samples
N	total number of items on test
P	probability of overall system
p	probability of component
U(t)	unavailability
R(t)	reliability
t	time
x	random variable
β	Weibull parameter shape parameter
λ	failure rate
η	Weibull parameter scale parameter
ω	failure occurrence rate

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Chapter 7
Optimization of an Integrated Complex of Process Plants and Evaluation of its Vulnerability

7.1
Introduction

The integration of a chemical complex is a development that has been undertaken for an extended period of time. The benefits are, clearly, the cost saving realized by a strong logistic situation (less transportation), mass and energy integration, and economy of scale. By the integration of process plants, a large demand is created at one location that drives to large, front-end process plants. External safety aspects that require large distances to be maintained between plant and domestic areas have driven the building of plants (specifically petroleum and base chemical plants) to be carried out at clustered locations. In the past, complexes were owned by one company, but with some add-on plants (e.g., oxygen plants). During the past few decades however, there has been a tendency to integrate process plants from different owners at a clustered location. In this respect, each company brings in its specific process(es), and these are integrated to obtain cost savings. In this discussion, no difference will be made with regard to the type of complex, which will be seen as a cluster of integrated processes.

The aspects of process integration at a complex to be discussed are:

- Development of design philosophies for integrated complexes:
- Selection aspects for a chemical complex
- Optimization of an integrated complex for mass flows
- Site utility integration
- Optimization of storage facilities
- Evaluation of the vulnerability of a clustered complex

In particular, the evaluation of site vulnerability is of major importance. Extensive integration with the objective being to save costs can make the overall system vulnerable. Evaluation of the site (complex) vulnerability will be based on reliability engineering techniques to quantify the likelihood of process outages over time. The total site (complex) vulnerability is expressed in terms of the product availability with opportunity gaps and a prioritized list of main contributors to the unavailability. This list is a good starting point for further optimization of design and operation of the complex. An additional factor in the design of a complex is that it is not a steady-state situation. Complexes are growing in size, and although there is a master plan (particularly for grass-root sites), this will always be subject to change. During the design of a complex, sufficient flexibility must be provided to cope with these uncertainties. Independent of these uncertainties in design capacity, there will also be operational variations among the different plants, and these need to be absorbed during operation of the integrated complex.

7.2
Chemical Complexes

Chemical complexes for base chemicals (which are considered as a global market) in general emphasize the existence of a certain production chain, and this depends on the activities of a specific company.

7.2.1
Nitrogen-based Complexes

These incorporate fertilizer-producing companies which, in general, operate a production train starting from natural gas (CH_4) and air to produce H_2, and N_2 with CO_2 as by-products. The chain continues with ammonia production (NH_3), from which extend nitric acid (HNO_3) and ammonium nitrate (NH_4NO_3) production. Urea (NH_2CONH_2) is also often produced in this scheme. [PB1]

7.2.2
Hydrocarbon-based Complexes

These are the producers of different types of plastics. Here, selected hydrocarbon feedstocks such as liquid petroleum gas (LPG), naphtha, and gas oil are converted into different products such as ethylene, propylene pyrolysis gasoline (also called pygas, a C_6–C_8 fraction) and a C_4 fraction containing butenes and butadiene. The C_4 stream may be fed to a butadiene extraction process for its recovery, while the remaining iso-butene can be converted to methyl *tert*-butyl ether (MTBE). Ethylene and propylene poly-olefinics are produced from the monomers. From pygas, benzene is recovered, and this may be converted with ethylene to ethyl benzene, next to styrene, and finally into polystyrene. Many other chemicals can be produced in this chain, including the co-production of styrene and propylene oxides from ethyl benzene and propylene, ethylene oxides, and ethylene glycols based on ethylene. For a typical flowsheet, see Figure 7.1.

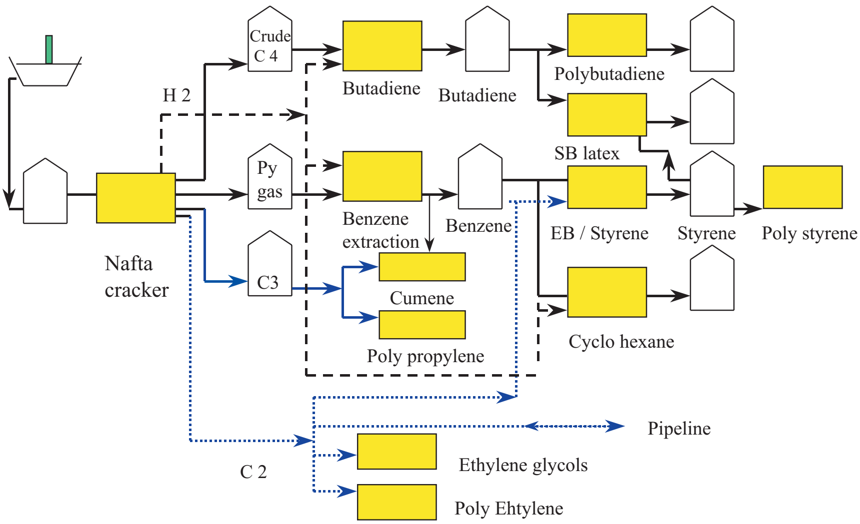

Fig. 7.1. An integrated hydrocarbon based chemical complex.

7.2.3
Chlorine-based Complexes

These are another example, and are at the front end of inorganic chemistry. Moreover, chlorinated methanes and other chlorinated hydrocarbons often also form a typical production chain.

7.2.4
Refinery Complexes

These are the most well-known application of integrated complexes that produce all kinds of fuels from crude oil. Different types of upgrading facilities are integrated into the refinery complex to obtain the maximum value from the crude oil.

Next to the above-mentioned product chains are those of the pharmaceutical and food industries. All complexes have their own typical set of processes, with unique levels of integration.

7.2.5
Combinations Complexes

There are also combinations of the above-mentioned complexes are also for example chlorine and hydrocarbons for the vinyl chloride monomer up and to PVC. Nitrogen and hydrocarbons complexes can form the base of aniline production, through the route of ammonia, nitric acid, nitrobenzene. The production of acrylo-nitrile from propylene and ammonia, ending in poly-acrylic nitriles, is another example of a production chain. A combination of refineries and hydrocarbon plants, for example in olefin production by cracking all kinds of refinery streams, is quite common. All the above complexes have product chains with forward and backward integration. If the customer product processes (e.g., polymer processes) form part of the complex, they depend heavily on specific markets and the distribution costs. Likewise, polyethylene processes are often sited at a larger complex due to the relative high distribution costs of ethylene. Latex and foam products are often produced close to the market due to the high transportation cost of the products.

The primary reasons for building integrated complexes are, first, to benefit from site logistics, where intermediate products can be moved from one process to the next at very low cost. In such cases, a dedicated line and a pump are often sufficient. Other benefits are achieved by taking advantage of energy integration with a site-wide utility system, while water integration and hydrogen integration might also be attractive options. Sharing facilities such as docks, rails, roads with (un)loading provisions can beneficial. One other advantage may be the utilization of intermediate product streams or side streams, which have a lower (mostly noncommercial) specification. These specific product streams are often much cheaper for the producing plant. The receiving plant might separate the desired material stream from its impurities at low cost, as that specific separation has already been provided in the process.

7.3
The Design Philosophies of Integrated Complexes

An integrated chemical complex has as its objective the achievement of lower production costs compared with that of isolated plants. This is realized by minimizing the logistics and processing cost of process plants, while maintaining the availability of the product streams at a high level. The vulnerability of such a complex requires careful quantification and evaluation to achieve the maximum benefits of integration.

In order to assure operational flexibility of an integrated complex, the following design philosophies are introduced:

- A failure or stop of a plant should not result in the immediate outage of other plants; this can be seen as clever integration on a site bases.
- The utility generation for a complex should be designed with an optimized level of redundancy, to minimize common cause failures of plants.
- Common cause failure of each utility system should be evaluated as part of reliability of the system.
- Simultaneous outages of more than one utility system should be avoided by designing the systems independently.
- The impact of utility outages should be minimized by the design of load-shedding systems; this might include power, steam, and others.
- The vulnerability of the complex should be quantified, and alternatives evaluated based on cost–benefit analysis.

Please note that one of the design philosophies for a process plant as discussed earlier is, "*Design for single reliable components unless justified economically or safety wise*". It will be clear that there is a difference between a process plant and an integrated complex, which boils down to the acceptability of a certain financial risk.

The reason for the above-mentioned site design philosophies is to avoid a chain of events, which may lead to a total or part site outage, as these involve a high cost. An immediate plant outage which results in an emergency stop (as in case of a total power failure) may cause different types of losses:

- Mechanical failures may occur due to the high temperature transients specific to this type of stop.
- Off-spec product(s) will be produced.
- Equipment may be blocked through polymerization or solidification.

Recovery from such stops can take considerable restart time (capacity loss) compared to a controlled stop. The above situations can justify an emergency power provision for certain subsystems, such as cooling water or a heating system. This can be considered as a third level of defense to name, in order of action: level of redundancy/back-up, load shedding system, and emergency provision.

7.4 Site Selection

Before the optimization and vulnerability of a complex is discussed, it is important to understand the technical aspects of site selection for the complex. It should be clear that site optimization is only a suboptimization compared to the selection of the site. In the past (and no doubt in the future), some sites have been totally phased out as the logistic situation was not sufficiently competitive in the global or regional markets.

The main aspects for site selection, although not all of equal importance, can have a major impact on the development and or economical operation of the complex. The selection aspects to be considered are:

- The process plants considered for the site are often part of a product chain(s), and will have to be subject to careful evaluation. The alternative options with (dis)advantages will largely be reflected in business studies and logistic studies (business studies are considered beyond the scope of this book). Any business partners or co-owners of the complex need to be identified. The selection of the site needs to incorporate these aspects.
- Develop a site mass and energy balance showing all process and utility streams between the plants and outside supplies. Such a balance will be subject to some iterations, but is necessary for a complete overview and to understand all interactions. Plants will not all be built and started at the same time, and therefore have to be scheduled in time. The balances have to be made available for all steps during evolution of the site.

- The logistic situation between raw-material supply at a global price and the product markets are crucial for the selection. Depending on the type of industry, some sites are situated close to the markets, while others have a relatively close access to raw-material suppliers. Half-way is often not the best location. The overall site balances will help in identifying the cost of all the material streams. The logistic study must include all modes of transportation: deep-water access, pipeline, railways, roads, and local waterways. For complexes projected inland, access to world market supplies can make the investment in relatively expensive pipelines a major requirement. Refineries situated inland need to have access to crude oil, and this will be one of the first comparisons to be made between optional sites and process plants under consideration.
- Individual plant overall mass and energy balances need to be prepared, complete with cost estimates.
- Utility cost and the availability of power, primary fuel, process water and cooling water are additional inputs for the logistic study.
- Utility plant design and energy integration potentials with the plants need to be identified, as they may have a significant impact on the utility cost. This must include any external supplies.
- Site logistic specifics; accessibility for transport over deep water, local waterways, railways, roads, and pipeline(s). The question to be addressed here is whether there any bottlenecks in these systems and, if any, will they be resolved. The constructability of plants also needs to be evaluated, for example soil research and the transportation of major equipment to the site.
- External safety and environmental requirements. Increasingly, global safety and environmental requirements are being applied. Thus, during the selection one should incorporate whether these are locally not yet at global level, and/or whether they will attain global status within the foreseeable future.
- Political stability.
- Permits procedures for building and operation of the complex might be inscrutable, and sometimes not achievable within an acceptable time frame. Some complexes were never built for these reasons.
- Economical environment, such as open or closed markets, taxes, profit management, and/or subsidies.
- The local culture and the availability of operational people. Another culture can be a severe handicap, particularly as this might lead to complete misunderstandings. In developing countries the availability of operational people must be carefully evaluated.

The above aspects have been listed as an overview of points for evaluation. As site selection has a high ongoing impact on the operational cost of the site, it was included in this chapter.

7.5
The Optimization of an Integrated Complex

The optimization of an integrated site is a balanced activity. On one hand, process plants can be designed totally independently of any integration, while on the other hand the site can be totally integrated and the system made totally dependent. The integration aspects are discussed where the right economic balance is the target for this activity. The discussion will be divided into:

- Site flowsheet with the corresponding mass balances and its variability.
- Site utility integration.

The integration will take place within the design philosophies, as discussed previously. Storage optimization and site vulnerability evaluation is discussed in the following sections.

7.5.1
The Site Flowsheet

7.5.1.1 Logistic considerations

The overall site flowsheet should be prepared to reflect the different processing plants. A plant is considered as a partially independent entity, characterized by a raw material storage up front and a product storage after the plant. These storage facilities might be shared by other consumers or producers, and often have loading and unloading facilities for import and export. A plant can have an intermediate storage tank in process for operational reasons; in that case the tank normally has only one supplier and one user and no (un)loading facilities. The site flowsheet must be completed with a site mass-balance. The individual plants can be subject to variations not only capacity-wise (as determined by the business), but also technically as catalyst aging or fouling might also have an impact. These last variations are however small compared to fluctuations as a result of market conditions. During operation, a difference in the site supply and demand balance will have to be solved by (un)loading facilities for the different (intermediate) products or provisions for external pipelines connections. The overall capacity for these provisions depends on the estimated imbalance by the businesses. Optimization of the storage facilities depends on the failure rates of the plant, the transportation volume, and frequency; reliability will be discussed in Section 7.6.

Of special consideration are the gas streams such as hydrogen, carbon dioxide, and fuel-gas as feed streams. In a similar way, this also applies to the utilities such as power steam, nitrogen, and air. These streams are, in general, all characterized by no storage facilities (very expensive), and can force a plant to an immediate stop as a result of a supplier outage. Different situations for direct supplies without any storage can be applicable:

- One plant specifically delivers this stream to one downstream plant; the stream then belongs to that plant, and the total plant reliability (including the supply plant) should be studied and used for decision making.
- The producing plant supplies the stream to other consuming plants:
  - The first option according to the design philosophy is to build a back-up facility such as a pipeline connection to an alternative source. For the alternative source, make sure that availability and reliability are part of the contract (be aware of all gas streams, steam and power supplies).
  - The second option is to design the producing plant at a very high reliability.
  - The third option is to build a load-shedding system to prioritize the consumer plants. This last option could be additive to the first two options. Load shedding is only applicable if there is limited availability.
- Shortage may occur in the supply and demand balance due to variable capacity operations of producer(s); in that case a back-up facility might be considered.

The site vulnerability study should include the gas feed streams.

7.5.1.2 **Lower-grade product streams for internal usage**

The potential of process streams between plants at a lower than commercial specification can sometimes provide a major benefit. The potential can be attractive technology-wise for components, which are difficult to separate in the upstream plant. In the consuming plant the product is often removed by reaction, and the impurity is concentrated and recycled to the upstream plant. A well-known example is that of the cumene (iso-propyl-benzene) plant. In this process, propane is recycled over the reactor while the conversion of propylene is 100%. The option to supply a lower-grade propylene, with propane as the major impurity, from a refinery off-gas or olefin plant can be very attractive for a grass root design. This option is also exploitable for an expansion project of the upstream plant, in order to avoid expensive investment. The back-up for these streams is mostly carried out with commercial grade product to avoid any additional storage for the lower-grade material.

Ethyl benzene plants have the ability to process lower-grade ethylene, with ethane as the major impurity. All ethyl benzene processes – the aluminium chloride route as well as the gas and liquid fixed bed, zeolite catalysed, routes – have this option (Netzer, 1997). The option of consuming lower-grade benzene in the ethyl benzene process is discussed by Netzer (1999), who presents the benefits of integrating ethyl benzene production with an olefins plant.

Other examples are the consumption of lower-grade styrene for poly-styrene, as well as the use of wet ethylene oxide for ethylene glycol production or wet butadiene for latex production. The removal of iso-butylene from a C_4 mixture is widely applied to the reaction with methanol to form methyl *tert*-butyl ether (MTBE).

Analyzing applications which might be attractive for the utilization of lower-grade reactants highlighted the following conditions as having potential for further evaluation:

- Products which are difficult to be separated from other components, but do not harm the receiving process. Examples include isomers (ethane/ethylene, propane/propylene, butenes) and benzene from a C_6 mixture of components.
- Consumer plants that achieve a high level of conversion; for example, ethyl benzene and cumene plants achieve a high conversion of olefins.
- Reactants which are diluted with components in the receiving process and were separated during up-front processing. Examples include the cumene process, where propylene is diluted with propane at the reactor inlet; the same applies to drying of ethylene oxide and butadiene before their use in respectively the ethylene glycol and latex plants. In the last processes the reactants are diluted with water at the inlet of the reaction.
- Reactants where additives are supplied for transportation or product stabilization and need to be removed in the receiving plant.

The use of lower-grade product streams is a major advantage at an integrated site, and can create considerable benefits. This, therefore, requires for creative thinking.

7.5.2
Site Utility Integration

Site integration takes place at different levels. The logistic integration and integration of mass flows by means of specific product grades were discussed above. Site utility integration in the past has mainly concentrated on energy integration, or more specifically heat integration. Currently, the integration is broadened to include mass flow integration.

7.5.2.1 Mass flow integration

The area of energy integration has been broadened during the last decade to water integration and hydrogen integration, and can be extended further to (generically speaking) mass flow integration. The pinch analysis technique evolved from heat integration representation with the temperature against heat duty in (grand) composite curves. As the quality parameter for heat, temperature was selected, while targets for minimum heat consumption could be easily determined (see **Chapter 4**). The extended pinch analysis techniques for integration of mass streams as water and hydrogen are based on representation of purity against mass flow, where purity or a specific contaminant is the quality parameter. The disadvantage is that multiple contaminants are difficult to handle during design. The analysis is similar to that of the heat integration technique. The target values can be determined and also upgrading steps (purification of streams) are comparable with heat pumps which are positioned across pinch points (Wang and Smith, 1994; Doyle and Smith, 1997; Serriere et al., 1994). The interest in mass transfer integration is growing. For water, it was the cost related to its scarcity, but also the cost of waste water treatment that were the drivers. For hydrogen, it was the scarcity which led to the need to design for minimum usage and upgrading of lower-purity streams, particularly refineries which have a growing shortage on hydrogen. The utilization of mass integration within a process plant was easy to handle with the traditional approach of "*look and see*", as the systems were small and the number of contaminants limited. For site integration, the system became complex due to the size and multiple contaminants, and this required a more structural approach.

The major concern with mass flow integration is that direct contact is created between different processes. In the case of heat integration, transfer of heat is through a heat exchanger, most commonly with a utility inter-medium. Direct contact may lead to process or safety problems which need to be carefully studied in each case, before this type of integration is applied. A preliminary safety study for these applications is mandatory. The use of lower-grade product streams with recycling of the impurities back to the supplying process (as discussed in Section 7.5.1) is also a form of mass flow integration. Also in that case, safety aspects with regard to process interaction must be reviewed up-front.

7.5.2.2 **Heat integration**

Heat integration of a chemical complex and its energy system is generally organised along the utility systems (Linnhoff and Dhole, 1993). The advantage is that by integration through utility systems a back-up becomes easily available, although it does not exclude direct integration between processes (see Figure 4.28 in **Chapter 4**). In general, that is applied for temperature level above 250 °C and between 80–120 °C, and at refrigeration levels.

In the design of a *site energy system*, a complex has a considerable steam and power demand; however, the steam to power ratio for different complexes is diverse. Herein, it is assumed that the complex has its own co-generation system for power and steam. On the other hand, the option to buy power and steam might be realistic. In the case of a low steam to power ratio (as will be the case with electrolysis processes), buying might be an attractive alternative, especially if a switchable contract is an option. For the discussion about the co-generation system it is indifferent if the unit is owned by an outside company or by the owner of the complex. There is a trend to buy steam and power from public utility companies, as these often operate at lower profit margins, as they have access to cheaper capital due to its lower financial risk.

The most energy-efficient way of energy generation with fuel is through a co-generation system (Figure 7.2). The design of such a system at a large complex is based on a gas turbine, driving a power generator. The off gases go to a waste heat boiler, generating high-pressure (HP) steam which, depending on the power/steam ratio, has additional firing. The HP steam is fed to back-pressure or extraction steam turbines which are sometimes equipped with a condensing turbine for operational reasons. The steam turbines drive is either used for mechanical power for process equipment such as large pumps, compressors or a power generator, but also smaller redundant rotating equipment to avoid common cause failures. Any imbalance shortage in the steam system is compensated by additional firing, and de-superheating let-down stations are provided. The connection between the different steam levels is shown in Figure 7.3. The heat exchangers, condensate headers and condensate flash drum are included. The number of steam levels depends on the specific

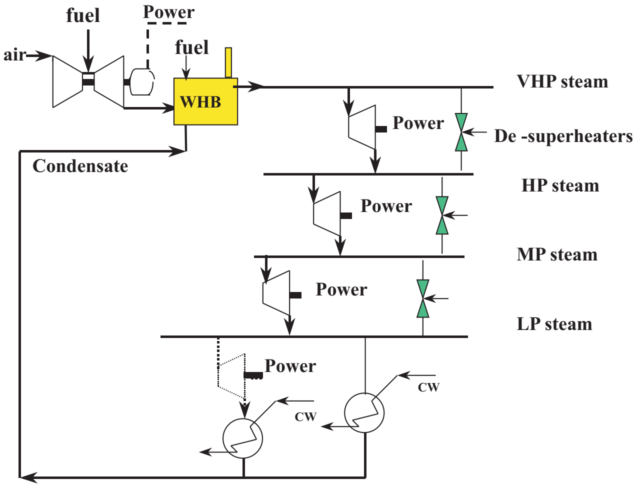

Fig. 7.2. Co-generation energy system.

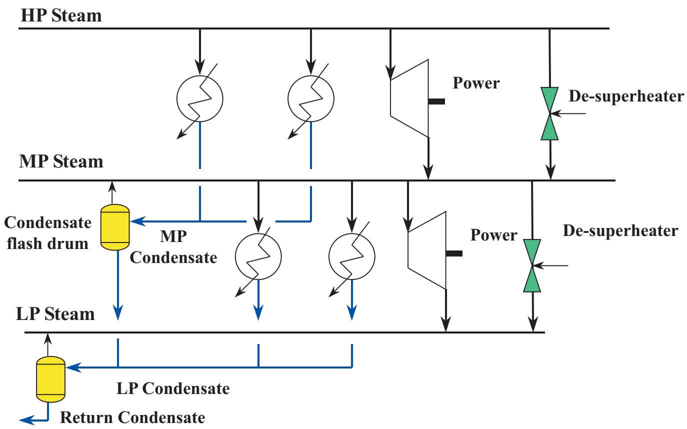

Fig. 7.3. Detail of steam header with turbine drivers, de-superheaters, heat exchangers and condensate collection.

demands of the complex, and form the basis for heat exchange between the plants. Smaller sites may have one or two steam levels, while larger sites have four utility steam levels. Smaller energy consumers may consider the application of a gas engines instead of gas turbines. The design of such an energy system is based on the input from the individual plants.

The *below-ambient temperature systems* (if applicable) are based on multi-stage compression refrigeration systems, the number of levels being determined by the consumers. The installation of an absorption system is very heat-intensive and only justifiable at moderate temperatures in the specific situation where we are certain that long-term, low-level heat is available at no cost. In general, they are applied in plants with excess low level heat in the 90–115 °C range.

For *grass-root sites*, the utility system and its levels have to be designed, and these are discussed in the following section. Existing sites have their utility energy levels selected, and process plants will accommodate the design of their internal system to these levels. After these energy levels have been selected, they are difficult to modify as the process equipment will be designed based on these temperature and pressure levels. The installation of an intermediate level locally (at plant) is practiced, especially if heat is generated and consumed at a level which lies between the utility levels.

The *individuals plants* should have made a pinch study and preliminary heat exchange network design of their plant (IChemE, 1997). An exergy study might also be useful to identify the situations where potentials for energy savings exist, to lower the energy targets by process modifications (Kotas, 1995). The information needed from the individual plant is as follows:

- The grand composite curves of the individual plants.
- The electrical power demand of the plant.
- The mechanical power demands of large processing machines potentially available for steam turbine or gas turbine drive.
- The availability of a furnace to potentially install a gas turbine or gas motor in front of (this will have an impact on the energy demand as this would exclude an air preheat on the furnace).
- The variations in steam and power demand due to process variability like capacity and catalyst aging, fouling.

A long-term energy forecast must be made for the site, based on projected projects. The accumulated information of the plants and the forecast will be used for an

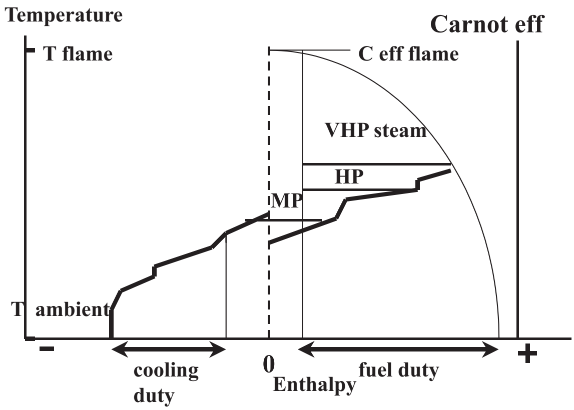

Fig. 7.4. Site sink and source profiles with steam levels (Ref. Dhole and Linnhoff with permission of Elsevier).

extensive evaluation of the site energy integration options and design of the energy system with its levels.

The *selection for the site steam levels* will be made by evaluation of the site source and site sink profiles, which are accumulated from the individual plant composite curves (Figure 7.4) (Dhole and Linnhoff, 1992). As was conclude earlier, in existing situations the energy levels have already been selected; in that case only expansions are under discussion, while changing the existing levels is in general not economical as the existing plants have already adapted their designs on the existing situation.

The most common solution is the selection of [none2] site steam levels with back-up from utilities, applied in the temperature range of 120–250 °C. The final result is a steam site balance which can be used for heat engine (steam turbine) selection.

On occasion. it may be beneficial to have an exchange of heat between individual plants (Ahmad and Hui, 1991). The exchange between plants mainly occurs through different intermediates, depending on the temperature levels:

- at levels above 250 °C with hot oil systems.
- between 80–120 °C with hot water or local steam systems (exceptionally with an organic medium).
- at temperatures below ambient, though the refrigerant.

The drawback is that back-up facilities needed to be available to guarantee independent operation of both partner plants, in order to meet the site design philosophy. The potential for cross-contamination of chemicals of the two plants encourages the use of a harmless intermediate for both plants. These must prevent any potential reactive chemical problem. The interaction between both plants due to heat exchange should not be underestimated in a design. The opportunities for exchange between plants are derived from the grand composite curves of the individual processes. When a plant has energy available at a temperature level which is close to the energy utilisation level of another plant, then the potential is there.

The selection of refrigeration levels is different from steam level selection, and is discussed in detail by researchers as Linnhoff and Dhole, 1992; Dhole and Linnhoff, 1994.

7.5.2.3 **Turbine drivers selection**

When a process furnace is an option for a gas turbine with power generator, this should be evaluated first as it has an interaction with the composite curves of the plant. The process furnace option should not necessarily incorporate a back-up for a failure of the gas turbine. Recall the plant design philosophy – "Design for single reliable components unless; economically or safety wise justified" (Koolen, 1998).

The potential of power (mechanical or electrical) generation by letting down steam to lower levels over steam turbines has to be exploited, as is foreseen in the co-generation scheme. The exploitation can in all practicality only be done once, so a choice must be made between the different options. In steam turbine driver selection, an inventory is first made of the requirements of plants for steam turbine drive. Large drivers are preferred, and especially those drivers which have a priority from a safety perspective such as a back-up cooling water pump drive for emergency cooling. Electric power generation driven by steam turbines with extraction at different levels is a generic solution. One disadvantage, however, is efficiency loss by conversion to electrical power and re-conversion to mechanical power for the drive of mechanical equipment. Before a selection can be made, the variability in steam consumption has to be evaluated.

The variability of in the steam system is not a shortage problem, as more steam can be generated and let-down systems are available. The concern is excess of steam at the lower steam levels.

Sites are also subject to fluctuation over time. These are caused by:

- Variable capacity operation particular of large, low-level heat consumers.
- Lower efficiency operation of processes as catalyst aging, lower compressor efficiencies or higher compressor load resulting in more lower pressure steam, through turbine drivers.
- Higher environmental temperatures, like during a day and night temperature cycle at summer conditions, resulting in more duty on turbine drivers.
- Upgrading of the process efficiencies at the site may result in less heat consumption particular at the lower levels.

The steam system should have the capability to cope with load variations.

The first rule always to be followed is: design the steam system with enough flexibility to avoid excess at the lower steam levels. Any excess has a high energy penalty. The options available for the steam system design are:

- Design with a structural shortage at the lower steam levels.
- Redundant mechanical equipment might respectively be driven by a steam turbine and an electric motor. The advantages are that the drivers can avoid a common cause failure. By this design the imbalance in the system can be manipulated by switching between drivers.
- Install steam drivers on steam systems which might fluctuate in load. The pronounced example is a electrical generator which easily can run on partial load. This can be specified at the design. A selected turbine driver might later on revamped by an other wheel configuration to better cope with a new condition in the steam system.
- Install a flexible condensing stage at the turbine drive which can benefit from any excess low-pressure steam by condensing operation.
- Design steam systems of plants rather independently, but at the selected site steam levels. This makes the plant less vulnerable, and also avoids the transfer of large steam flows over the site. This is also applicable for steam turbine drivers, as these are often selected and are preferably closely situated to a steam-generation facility.

The evaluation and selection of the turbine drivers alternatives must be completed. Now, the site and process steam balances can be prepared, including all turbine drivers.

7.5.2.4 Utilities availability

The sensitivity of the site utility system has a major impact on the vulnerability of the site. Therefore, an evaluation of availability of the site utility systems requires a careful quantitative basis. A trade-off must be made between investment cost for redundancy/ back-up provisions versus the quantified risk of production losses. The availability calculations should be done in the same way as for the plants (see Section 6.4 in **Chapter 6**).

The involvement of the availability of external supplies must be included. During this study, the load-shedding options need to be explored and prioritized, and specific attention must be given to common cause failures. This goes beyond the study as described in Section 6.4, which assumed no common cause failures of the individual steam generators.

The output of the utility reliability and availability must be used as input for the site vulnerability study (see Section 7.7).

7.5.2.5 Summary utility integration

The design principles for heat integration at the site are:

- All plants must have a pinch analysis and heat exchanger network design.
- The optimal energy system for a complex based on fuel is a co-generation system for power and steam.
- Heat integration between plants is preferably done through a utility system, but in case of direct exchange the philosophy of independent operation of the plants must be respected.
- A quantitative reliability study must be available for the utilities, with a thorough analysis for common cause failures of utility generators. This study needs to include the reliability of the different load-shedding levels for applicable utilities such as power and steam.

7.6 Optimization of Storage Capacity

The optimization of the storage capacity will be illustrated through analyzing a tank, which is located between two processes (Koolen et al., 1999; Mihalyko, 1999). In this particular example, the tank has only one inlet stream from the upstream process and one outlet to the down stream process (Figure 7.5). The size of the tank must

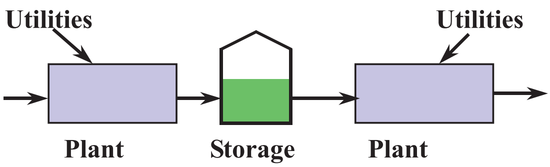

Fig. 7.5. Optimization of storage capacity.

be optimized versus the loss of production due to failure of the upstream and downstream processes. The production loss of the downstream plant is what counts, as that material is not available for further processing or sale. The example is used to illustrate the calculation method, but it can be extended to any storage provision in a supply chain.

7.6.1 Plant Failures

The first steps that must be taken are the quantification of the failures; this is also expressed as the *unavailability* of both processes, upstream and down stream (Shorr and Griffin, 1991). The availability of plants can be divided into *mechanical availability* and *process availability*, including planned stops.

The mechanical availability of the plant is affected by its components with their own typical failure rates and distribution, and can be quantified with a reliability engineering technique. It can be simulated with a software flowsheeter, which is provided with a random generator (Malchi Science, Clockwork Design). The plant is divided into components or a set of components of which the failure rates and their distribution must be collected. There are different sources for these data, there are several public data banks (e.g., CCPS, Oreda), and data banks of equipment suppliers. Processing companies may also have their own data banks. Besides failure data, repair times and process recovery times (start and stop times), together with their distribution, are also required. The last data are collected for the process under study from maintenance and plant data. The utilities and supplies of the process also are analyzed for their failure rates. The individual components or set of components are implemented in a flowsheeter and simulated as a set of serial and parallel components with their specific properties. The simulation with its random generator runs for an extended time (called the *mission time*), and for a number of runs. After a sufficient number of simulations, the results will converge to a set, with limited variation. The results may be expressed in several ways as: the total number of stops per year; the average duration of these stops and its distribution; the downtime per year; the number of stops per type of components and its spread. The overall results give the plant mechanical failure rates and its distribution. The technique can be used to compare several process alternatives that affect the reliability of the design, and there will be a trade-off between production increase and capital. The best economic alternative will be a preferable choice as bases for design. For details on the reliability methodology for process design, see **Chapter 6**.

The plant mechanical failure rates must be complemented with the process failure rates. Process failures might be caused by fouling, catalyst degradation, and operational failures. The process failures are sometimes covered in planned stops (in which case it is not seen as a failure), but it will be included in the overall availability. The data for process failure rates can only be collected from careful analysis of process data over the past. These data become more accurate if more historic data are available. Licensees of the technology sometimes collect these data for their specific processes. The overall plant failure of both process and mechanical failures have an impact on the sizing of the storage tank. Planned plant shutdowns are excluded from this study as it is assumed that during that time period special measurements are taken to cope with storage provisions internal or external.

7.6.2 The Storage Tank

A storage tank design study is limited in this example to an intermediate storage tank between process sections, as discussed in Section 6.4 in **Chapter 6**. The tank is placed between the upstream and downstream process, and is simulated as a volume with a certain capacity. A clock is implemented in the flowsheet model, and a capacity set point for each process is determined. During the simulation in time we now calculate the inlet and outlet streams of the tank based on the actual capacity flow over a time interval. The tank hold-up is determined at time intervals by balancing the input and output streams of the tank. The tank is provided with a simple level controller which manipulates the capacities of the upstream and downstream processes to a definable algorithm. It functions in this example as follows.

The level of the tank is planned to be between 45 and 55% at balanced operation; say its set point range is 45–55%. The capacities of both processes are put at 100% at the start of the simulation, as the size of the tank is determined at design capacity. When the level of the tank is between 55 and 95%, the capacity of the downstream process is put at 105%, and that of the upstream process at 95%, to bring the tank level back to the 45–55% range. When the tank is between 5 and 45%, the capacity of the upstream process is put at 105%, and that of the downstream plant at 95%. Now, the level goes up to 45–55% range. When the tank is at 5% level (nearly empty), the downstream process is switched off (zero capacity); at 95%, the tank is

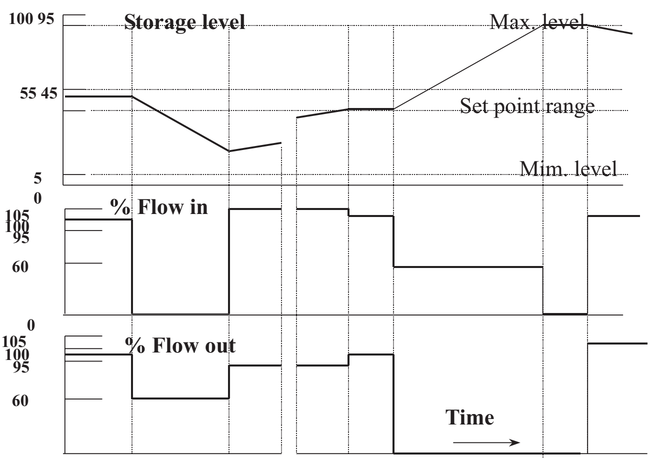

Fig. 7.6. Histogram of feilures and effect on level and flows.

nearly full, and so the upstream process is switched off. In case of a process failure, the processes in the production chain are set at 60% capacity. The above discussed level controller affects the capacity controllers of the processes. The level controller might be designed in a more sophisticated fashion, but for the purpose of the example it was considered sufficient. A qualitative histogram of storage tank level and the related inlet and outlet flows is shown as result of failures in Figure 7.6.

The *assumptions* for this study are that:

- the process runs for five years between turn arounds, which is equal to the selected mission time.
- an intermediate process stop is planned every two-and-a-half years for 1 week.
- utility availability is 1.0.
- the availability of raw material is not a constraint.
- product delivery does not constrain the production.
- the storage capacities under evaluation (expressed in hours of maximum throughput) are: 0, 10, 18, 20, 24, and 36 hours.
- the set-point range for storage is 45–55%.
- the capacity throughput alternatives as a percentage of maximum capacity are 0, 60, 95, 100, and 105%.
- the number of simulation runs were limited to 60 histories, and this causes some variation in the results. An increase in the number of simulations would have narrowed down the variability.
- the minimum repair times were set at 12 hours based on organisational constraints. All small rotating equipment was reparable or exchangeable within 12 hours.

7.6.3 Simulation and Results

With the tank and its controller implemented in the RDB (reliability block diagram) flowsheet between both processes, we now are able to simulate the whole configuration. The processes may be described as a combination of individual components, or as overall plant failure rates deduced from its components. The system is now subject to probabilistic simulations with a Monte Carlo generator for the variables (as was described for the individual process reliability studies in Section 6.4 of **Chapter 6**). In the example, the upstream and downstream processes are described as a combination of serial and parallel components. This explains, in combination with the limited number of runs, the variation in mechanical failure results (number of stops and down-time).

The results can be presented in different formats and might emphasize:

- The number of process stops per year.
- The down-time in hours per year (both the down-time and number of stops can be specified per component and totalled).

- The number of stops due to full or empty tank situations of respectively upstream and downstream processes.
- The down-time as a result of full or empty tanks.
- The variation in tank level over time.
- The process (un)availability of upstream as well as downstream processes, in % of time or hours per year.
- The process capacity in % of maximum capacity, calculated by summation of the production intervals production capacity over mission time.

Through multiple simulations for different levels of process reliabilities and storage capacity, the impact of these variables are obtained on process performance. It should be noted that the results of the downstream process are mandatory for the production performance, as it is here that the ultimate product is delivered.

The results for the upstream and downstream process are presented in Tables 7.1–7.4. The following observations can be made from these data.

Table 7.1. Reliability and unavailability of upstream process (Figure 7.5) and the impact of storage capacity.

	Storage capacity 20 h	*Storage capacity 24 h*	*Storage capacity 36 h*
Low process reliability			
No. of mechanical stops/year	6.47	6.32	6.62
No. of times tanks full/year	1.64	1.44	0.76
No. of total stops/year	8.11	7.76	7.38
Unavailability (h/year)			
by mechanical failures	124.08	117.46	109.94
Medium process reliability			
No. of mechanical stops/year	3.59	3.72	3.75
No. of times tanks full/year	1.49	1.51	0.73
No. of total stops/year	5.08	5.23	4.48
Unavailability (h/year)			
by mechanical failures	89.30	91.46	79.24
	Storage capacity 10 h	***Storage capacity 18 h***	***Storage capacity 24 h***
High process reliability			
No. of mechanical stops/year	2.24	2.35	2.24
No. of times tanks full/year	2.93	1.59	1.35
No. of total stops/year	5.17	3.94	3.59
Unavailability (h/year) by mecha-			1.14
nical failures	92.04	74.82	66.93

Table 7.2. Reliability and unavailability of downstream process (Figure 7.5) and the impact of storage capacity.

	No storage	*Storage capacity 20 h*	*Storage capacity 24 h*	*Storage capacity 36 h*
Low process reliability				
No. of mechanical stops/year	4.86 + 6.47*	4.86	4.92	4.92
No. of times tanks empty/year	–	1.39	1.01	0.28
No. of total stops/year	11.33	6.25	5.93	5.20
Unavailability (h/year)				
by mechanical failures	191.58	108.8	106.8	99.98
Medium process reliability				
No. of mechanical stops/year	3.52 + 3.59*	3.52	3.55	3.51
No. of times tanks empty/year	–	1.40	1.08	0,27
No. of total stops/year	7.11	4.92	4.63	3.78
Unavailability (h/year)				
by mechanical failures	136.47	91.64	92.11	82.71
		Storage capacity 10 h	*Storage capacity 18 h*	*Storage capacity 24 h*
High process reliability				
No. of mechanical stops/year	2.97 + 2.24*	2.97	2.82	3.01
No. of times tanks empty/year	–	2.12	1.37	1.02
No. of total stops/year	5.21	5.09	4.19	4.03
Unavailability (h/year)				
by mechanical failures	118.71	99.45	83.72	80.09

* Summation of mechanical stops of upstream and downstream processes.

Table 7.3. Overview of process stops by tanks full or empty situations of respectively upstream and downstream plant for different process reliability levels at different storage capacities.

	Storage capacity 20 h	*Storage capacity 24 h*	*Storage capacity 36 h*
Low process reliability			
No. of tanks full	1.64	1.44	0.76
No. of tanks empty	1.39	1.01	0.28
No. of tanks total	3.03	2.45	1.04
Medium process reliability			
No. of tanks full	1.49	1.51	0.73
No. of tanks empty	1.40	1.08	0.27
No. of tanks total	2.89	2.59	1.00
	Storage capacity 10 h	*Storage capacity 18 h*	*Storage capacity 24 h*
High process reliability			
No. of tanks full	2.93	1.59	1.35
No. of tanks empty	2.12	1.37	1.02
No. of total tanks	5.05	2.96	2.37

Table 7.4. Overview of down-time of downstream process (hrs/year) for different process reliability levels at different storage capacities.

Process reliability level	*No storage*	*Storage 10 h*	*Storage 20 h*	*Storage 24 h*	*Storage 36 h*
Low	191	–	109	107	100
Medium	132	–	92	92	83
High	119	99	84*	80	–

* Data from 18 h storage capacity.

- The mechanical stops for the different reliability levels show some variation (the number of mechanical stops should be independent of storage volume) (Tables 7.1 and 2). Compare the results of the number of mechanical stops on a horizontal line. The reason for the variation is that the processes were modeled at component bases, while the number of simulations were limited. By extension of the number of simulations the results would converge to average values with less spread.
- The number of mechanical stops in time are a good indication of process reliability.
- The number of mechanical stops for the downstream process is much higher for a combined process without any intermediate storage compared to processes which are separated by storage. This can be concluded from the total number of mechanical stops with and without storage in Table 7.2. Compare the number of stops per year for "medium process reliability", which for a no storage situation are 7.11, and for a 24-h storage facility 4.63. Similar results are obtained for the processes of different reliability levels.
- The capacity of the intermediate storage tank has a clear impact on the number of process outages. The number of stops caused by a tank being full or empty are summarized in Table 7.3. Comparing the data for a low reliability process shows that the number of stops decrease from 3.03 to 1.04 when the storage capacity increases from 20 h to 36 h. For the medium reliability process, the decrease in number of stops in relation to storage capacity has the same ratio. For the high-reliability process, the same trend is observed, although these data are not directly comparable as different storage capacities were used.
- The total down-time of the downstream plant, which sets the ultimate capacity, is clearly affected by the storage capacity (see Table 7.4). Comparison of the data for the same process reliability level shows a reduction in down-time with an increase in storage capacity. For a high-reliability process the down-time decreases for no storage versus a 36-h storage from 191 hrs to100 hrs. At higher process reliability levels, the effect is less pronounced.

The above data are to be used for a cost–benefit analysis of capacity loss and operational losses versus investment to obtain an optimal process. The process alternatives to be evaluated are process reliability, as well as storage capacity.

7.6.4
A Chain of Production Processes

A chain of production processes with intermediate storage capacities are quantified in the next example (Figure 7.7). The type of processes are not really relevant. What is specific in this example is that several plants are in series, while a waste treatment facility was included with its buffering capacity. Another specific is that there is no intermediate addition or removal of intermediate products. The transportation of the final product by railway included, the trains being planned to run twice weekly (Monday and Thursday), with 24 h reserved for loading. The loading has been included in the model, while the reliability of the transportation system was assumed to be 1.0. This means trains always arrive in time, and the train needs to leave on time to meet the reliability of the transportation system. The maximum capacity of the train is fixed.

The waste treatment process played a crucial role as the process plants had to stop in case of a waste tank being full; thus, it was treated like a successive process. The amount of waste of process A was very small in comparison to the other processes. It was assumed that the waste treatment process would not have a direct effect on process A. Therefore, a connection was not foreseen in the model.

The assumptions made for this situation are identical to the previous example of the intermediate storage tank:

- The utility reliability is set at 1.0.
- Raw material is available.
- Product receiving is not a constraint.

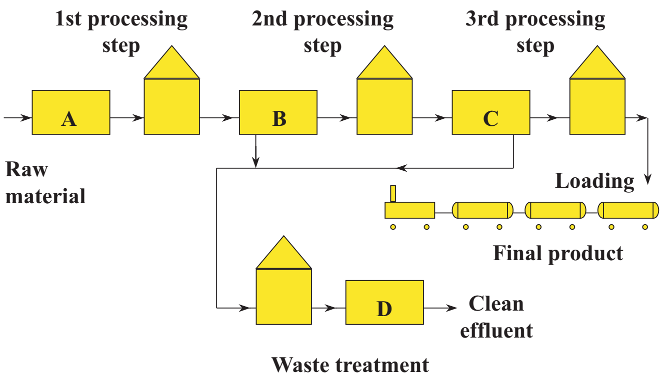

Fig. 7.7. Chain of production processes with intermediate storage and waste treatment plant.

- Mission time is 5 years, and the number of simulation runs was 60.
- The level control of the intermediate tanks was identical to the previous example, with the set-point at a range of 45–55%.
- The storage capacity was widely varied.
- Capacity flows were 0, 60, 95, 100, and 105% of maximum capacity.

7.6.4.1 **Simulation results**

The simulation results are summarized to show the impact of the storage capacities. The simulation of supply chains for optimization can among others also be solved with software named "Arena" from Systems Modeling Corporation. The reliability level for the individual units varied, but for illustration of the storage capacity effect these data were limited to one set. The availability of the individual units is listed in Table 7.5.

The individual processes have different availability and failures in time, as can be concluded from the data. Each process has its own configuration, and therefore its specific availability and failure rates. The availability of the waste treatment process is very high and its failures very low. Only once in 7 years did the waste treatment fail mechanically. The summation of mechanical failures of the four processes is 26.7 per year), which can be considered as high.

The impact of storage capacity on overall process performance is quantified as % of production capacity in Table 7.6. In comparing the data, it can be seen that no storage gives the lowest capacity (95.5%), compared with 98.0% for 24-h storage and 99.0% for a very long storage of 900 h.

Table 7.5. Availability and failures of individual processes.

	% Availability in time	*Failures per year*
Process A	98.4	10.03
Process B	98.6	9.83
Process C	99.0	6.70
Process D	99.6	0.14
Total		26.7

Table 7.6. Capacity of overall process at different storage capacity.

Storage capacity (h)	*% Capacity of final product*	*Process failures /year*	*% Partial filled trains*
900	99.0	26.8	
24	98.0	34.6	4.7
0	95.5	27.6	

It can be concluded that, in this case, a rather small storage gives an increase in capacity of 2.5%. The total process failures show a spread, although the failures should not be affected by storage capacity. The spread is caused by the same reason as discussed previously. For the storage capacity of 24 h, the number of trains that were partially loaded were counted and expressed as % partially loaded trains. These are only summarized data. Many details might be obtained, as was illustrated in the previous example. To mention some of these, a ranking can be made of causes of failures and down-times, including tank-empty and tank-full situations. The level of storage can be plotted over time. The methodology applied in this case did not differ from the previous example in this section – only the size of he problem was increased.

The variables for such a chain of production facilities are: process reliabilities and availability; storage volume of each intermediate tank; set point of the level in storage; and transport reliability and availability. The set point of storage level is important when the availability of the supply and receiving streams shows a large difference.

The last example can easily be extended with transportation data of raw material, but also with supply and delivery requirements. Intermediate product streams might be loaded or unloaded and can be included in the scope. Particular options for supply and delivery requirements might be the subject of further study. This makes the cost of these (mostly contractual) terms viable, and enables the settlement of an agreement on optimal terms for both partners.

In conclusion, one can say that reliability studies are an excellent tool for the determination of the impact of process reliability and storage capacity on production availability and capacity. The data form a sound basis for a cost–benefit analysis of investment in this field. In the next section, the extension to a supply chain at a site is discussed.

7.7
Site Vulnerability

The objective of a site vulnerability study is to identify weak points in the infrastructure of a complex which could lead to an unacceptable level of unplanned partly or total outages and related losses (Figure 7.8).

Economic criteria can be applied when the losses that may occur during an outage can be quantified in relation to the investment cost to reduce them. The order of magnitude for a chemical complex experiencing a total unplanned outage might be once every 20 years. This depends a great deal on the availability and failure rates of utilities. It must be clear that specifically for power, one might have a large availability but still a large number of relatively short power losses. It is the number of these power losses which sets the stage in such a case. For a plant, an unplanned outage may occur somewhere between a few times per year or even less, and this largely depends on the design of the plant. A quantitative method is shown here of how to determine the vulnerability, and ways in which it can be improved. This avoids the

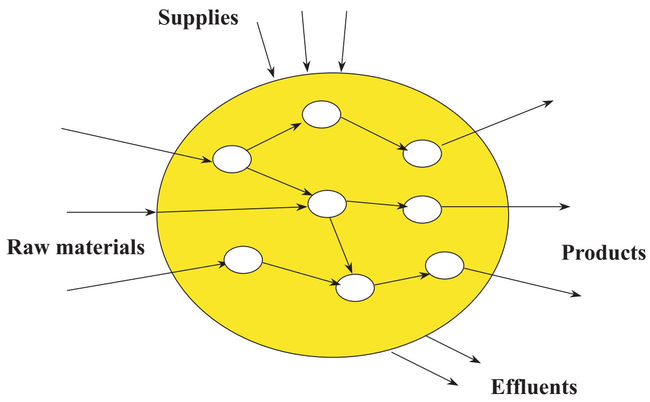

Fig. 7.8. Site vulnerablility???

introduction of site design policies that are always expensive. The methodology is applicable for existing and new complexes, while updating can also easily be carried out (Koolen et al., 1999).

The methodology for a *vulnerability study* is presented below.

- A flowsheet is developed which contains all the process plants placed in a sequential and parallel order, as shown for a hydrocarbon-based site. For a typical hydrocarbon-based complex, the hydrocarbon cracker plant is the basic process (see Figure 7.1). For other integrated complexes such as a refinery, the basic process is the crude distillation. For a nitrogen-based complex, the synthesis gas plant and its adjacent NH_3 plant are the basic process. The flowsheet starts at the raw material transportation that is considered as a processing step. Raw material storage and the basic process of the manufacturing chain are next. Then we pass through all processing steps of the supply chain to the final plant that makes the product, which is transferred outside the complex. They are represented as a RDB, as used for reliability studies. The diagram is a line diagram with serial and parallel components, as discussed previously in **Chapter 6**. The processing steps are shown as blocks, and separated by storage facilities if available. The intermediate storage facilities might be equipped with loading and unloading facilities to cope with any imbalance of the site mass balance.
- The complex overall flowsheet (RBD) is divided into supply chains. An example is shown of C_4 and C_6 supply chains in Figure 7.9. The utilities are not shown on the diagram, but are implemented in the simulation as separate streams to the plant blocks. All relevant mass or energy streams are shown when they come from another plant, or from outside the complex. In case a liquid stream comes from a storage facility and the stream is only small compared to the main stream is assumed as not relevant. By comparing the capa-

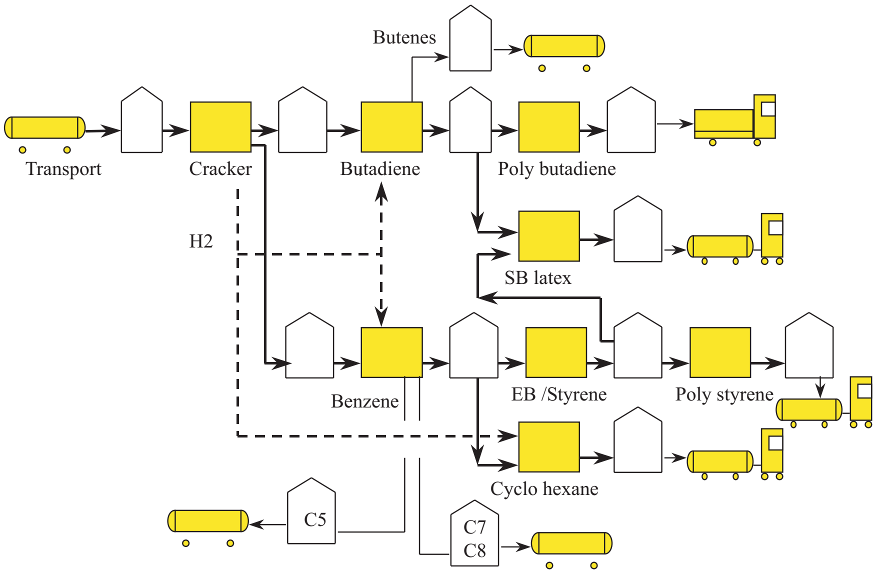

Fig. 7.9. Reliability block diagram for and C4 and C6 chain of hydrocarbon complex.

city of the processes, the styrene flow to the latex process might be small and considered not relevant compared to the main styrene stream. In the overview of the site (see Figure 7.1), the hydrogen streams for three downstream plants are clearly shown, as in this situation they are all relevant as they can lead to immediate outage of several processes. For a hydrocarbon-based integrated complex the flowsheet can logically be split into C2, C3,C4, and C6 supply chains. It should be noted that each supply chains always start with the import of raw material and the basic process. An independent process on the complex (not linked to the basic process) can be treated as a separate supply line although integration on utility level still creates a potential vulnerable situation.

- The determination of the individual plant failure rates as mean time between failures (MTBF) with its distribution and recovery times is the next sequential step. This may be done by a component analysis (as described earlier) or through analysis of the plant historic data. We should assure ourselves specifically in the last case that we have sufficient data from which to draw conclusions.
- The availability and failure rates of external supplies such as power, fuel gas, and hydrogen. The failure rates of all individual utility systems such as power, steam, cooling water, nitrogen, and fuel gas have to be determined based on component data. The hydrogen system is treated in a similar way,

though strictly speaking it is a raw material. The load-shedding systems need to be included with its shortage levels. The frequency of load shedding at the different defined shortage levels must be determined based on the reliability of the utility system. The selected process plants to be switched off when load shedding levels becomes activated must be known These supplies have a major impact on site vulnerability, and therefore require an optimal balanced but high availability and reliability.

Factors playing a role in the achievement of optimal (but high) availability and reliability for common (utilities) supplies include the following:

- Availability
  – Reliable design
  – Inventory to cope with temporary shortage
  – Back-up to cope with longer shortage times, or when inventory is not practical, as for power and gases such as hydrogen
  – Load shedding to minimize the impact
- Reliability
  – Reliable components
  – Reliable supplies
  – Redundancy
- Common mode failure
  – Independent systems
  – Different designs
  – Independent external back-up
  – Inventory
- Emergency provisions
  – Independent system (emergency generator, diesel driven firewater pumps)
  – Inventory (firewater pond, oil reservoir, batteries)

All the above factors require careful design as they have a major impact on site vulnerability. In the previous chapter reliability engineering techniques were discussed which resulted in availability and reliability process data. For (utility) supplies, common cause failures have an additional importance in the prevention of outages.

The Center for Process Safety (CCPS) in Chemical Process Quantitative Risk Analysis (CPQRA) book (1989) mentions that: "... common cause failures events tend to dominate system unavailability in those applications where redundancy is used to improve system reliability performance". Therefore, the reliability calculation method needs to be adapted to quantify its impact. A methodology has been developed reported in CPQRA to perform a common cause failure analysis to support designs. The basic elements of this are:

– Identification of common causes for events.
– Building of common cause event trees.
– Qualitative screening for the selection of dominant contributors to system unavailability.
– Quantitative analysis by common cause event modeling.

- A *parametric technique* is often applied which is called the Beta Factor model (Mosleh et al.,1988). This techniques introduces for each component an independent failure rate and common cause failure rate:
  $\lambda = \lambda_i + \lambda_c$
  λ = component failure rate
  λ_i = independent component failure rate
  λ_c = common cause failure rate
  The beta factor has been defined as $\beta = \frac{\lambda_c}{\lambda_c + \lambda_i}$

This approach assigns high failure rates for similar redundant systems.

- *Quantification* of a common cause event tree is a more fundamental approach, which generates more realistic data:
- – Analysis and evaluation of alternatives for improved design

The above addresses common cause failures for a utility supply.

The prevention of losses of two or more utility supplies at the same time is of even greater importance, as this can lead to high losses. This can only be adequately realized by independent systems. A positive example is that of a redundant co-generation system where a gas turbine drives a power generator with waste heat boiler for steam generation, while extraction air from the air compressor is dried and used as instrument air. Such a system is independent as it generates its own power, steam, and air. An assured boiler water supply is still a requirement which is in general realized by sufficient storage. An overview is given of practical measures for utility systems in Table 7.7.

Continuation of the methodology for site vulnerability evaluation brings us to:

- The transportation mode failures and its distribution of raw materials and products, eventually completed with any delivery or supply requirements.
- The capacity of the storage facilities.
- Modeling; the collected data are all input for the reliability simulation model that is based on the RDB, as discussed previously. Each applicable utility must be connected to the individual plant blocks (Figure 7.10).
- A base case for the complex is simulated for the existing or planned situation.

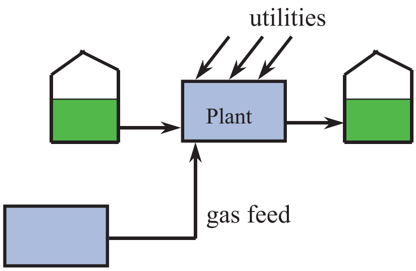

Fig. 7.10. Plant block with basic connections.

Table 7.7. Measures practiced to achieve reliable utility supplies.

General
- Utilities systems should operate as independently as practicable in order to avoid the loss of one utility causing the loss of another.
- The power supply for utility systems should have the highest priority for supply through the load-shedding system
- Emergency systems should be totally independent
- A quantitative common cause failure analysis is a requirement for utility systems

Power supply
- Redundant power generators executed as independent systems*
- External back-up with redundant transformers and supply lines
- Inventory, limited to power for instruments on batteries
- Load-shedding system
- Emergency generator driven by combustion engine

Steam supply
- Redundant steam generators executed as independent systems*
- Boiler feed water inventory
- Redundant feed pumps with different drivers (electrical, steam)
- Redundant de-superheaters
- Load-shedding system
- Emergency provision locally electric heating

Air supply
- Redundancy on compressors executed as independent system*
- Separate drying units per compressor set
- Different types of drivers for compressors
- Separate power supplies for drivers
- Back-up from air compressors of gas turbines with dedicated drying units

Hydrogen supply
- Alternative sources
- Purification and compressor systems single due to high reliability
- External back-up preferable at specification to obtain redundancy for purification and compressor system
- Load shedding

Process water
- Inventory tank/pond
- Redundant pumps with different drivers (electrical, steam)
- Redundant power supplies

Demineralized water
- Inventory of demineralized water
- Redundant pumps with different drivers (electrical, steam)
- Redundant power supplies

Cooling water system (centralized)
- Cooling water circulation pumps redundant with different drivers (electrical, steam)
- Cooling towers with more cells
- Redundant power supplies
- Emergency cooling with independent fire water system driven by combustion engine

* For power, steam and air supply, gas turbines with waste heat boiler and air compressor can be designed totally as independent systems.

Evaluation is the most important step that already starts during the collection of the input. It is not the intention here to provide specific data, but rather to emphasize the important factors for evaluation.

- The flowsheet already shows the critical material suppliers, those that do not have a storage facility like, hydrogen, fuel gas, power are subject to special attention.
- The failure rates of the utility systems or fuel gas supplies set the basis for total complex outages. Careful study can give surprises, such as the relevance of a reliable water supply, and others. Electrical power is always of concern, as the availability might be high, but a high frequency of short interruptions leads to frequent load shedding (losses). Utilities that do not activate a load-shedding facility and are essential for the majority of the plants should have a high MTBF, in the order of 50 000–100 000 h.
- The failure rates of the plants provide a good insight into specific plant reliability, and might ask for a detailed component analysis to evaluate the reliability. The base case of the simulation shows the impact of different components on the final product availability. These can be tabulated and prioritized as function of down-time and number of outages, in the same way as is carried out for plant reliability studies. The priority list may contain the following elements: the plant's unreliability; storage tanks full and empty; utility per item; and external feed interruptions. This provides a clear insight into the main contributors.

Based on the availability data of the final product streams, the opportunity gap can be quantified in money terms. These potential benefits are the bases for economic evaluation of process alternatives for reliability improvements as; external supplies, plant(s) reliability, storage capacities, load-shedding systems, redundant generation, or back-up for direct feeds (feeds without storage).

Next to the evaluation of design alternatives to optimize the availability of an integrated complex, this will also provide data to optimize the operation. The operational set point for the storage tanks can be optimized.

7.8 Summary

- Site vulnerability is mostly approached by the application of policy rules, which leads to over- or under-investment in logistic and utility provisions.
- Currently, reliability engineering techniques enable the simulation of a site from import of the raw materials up to delivery of the final products. These studies are applicable for new as well existing situations. Modification of the site (and in particular of the utility systems) would justify upgrading of the reliability study.
- The following facilities are a degree of freedom for vulnerability studies:
  - Individual process reliability

- Storage capacities
- Utility supplies reliability and availability

- A step-wise methodology has been described for a site vulnerability study. For a large integrated complex, the problem is split into supply chains.
- The utility supplies play a dominating role in site vulnerability. A detailed reliability study must be performed for each utility and gas supplies such as hydrogen, based on component analysis. For utility supplies, common cause failures tend to dominate the unavailability where redundancy is used to improve system reliability. The methodology to identify and quantitatively incorporate common cause failures in the reliability study is referred to.
- The results of the site vulnerability study can be presented in a prioritized list of contributors to unavailability and outages over time.
- Evaluation of alternatives makes a cost–benefit analysis possible, and forms a good quantitative basis for site investments.

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Chapter 8
Instrumentation, Automation of Operation and Control

8.1
Introduction

Simple and robust process plant design is a concept, which includes hands-off operation (Koolen, 1994). Earlier in this book, the objective for such a plant was defined as:

An optimal designed safe and reliable plant, operated hands-off at the most economical conditions

The introduction of simple and robust process plants must fit into an evolutionary cycle. Simple and robust is something which is from all ages, but a technology has still to grow to a certain maturity before its wider application can be achieved. Preconditions regarding the technology for a simple and robust process plant as defined are:

- The technology needs to be understood and to be quantifiable.
- The equipment needs to meet criteria for reliability and robustness.
- Instrumentation must be reliable and robust.
- Operation must be automated.
- Control of the operation must be designed to be robust.

It is the evolution in instrumentation, automation and control technology that has made such tremendous progress during the past few decades. Initially, this was through the evolution of computer and communication technology, during which time instrumentation went from pneumatic through electronic, single loop instrumentation to multi-loop instrumentation systems equipped with computers and fieldbuses.

Instruments were made more reliable and robust, including process analyzers; indeed, recent analytical instruments have become more reliable even than laboratory measurements. Instruments now have self-diagnosis systems, while analyzers are equipped with self-checking and calibration provisions.

Based on the progress made in instrument reliability and robustness, the following design approach becomes applicable to simple and robust plants:

better have few good reliable instruments than lots of unreliable ones.

Simple and robust plants minimize on instrumentation versus conventional design; in other words, fewer components results in fewer failures.

The automation of processes to operate consistently by minimizing human operation is applicable based on reliable, robust instruments and instrumentation systems and provided with robust operational programs.

Robust control must meet the criteria of hands-off operation; this means that the operator is not in the control loop, although in most processes this is not yet a reality. The control technology is on the brink of major change. Currently, the basic process control is based on heuristic rules for the selection of the control strategies. The design of predictive or model-based controllers (multi-variable controllers) to enable operation at its constraints has been developed during the past decades. The design of these controllers is based on linearized input and output models around working points. These models have been developed with process identification techniques on existing processes.

The technology of dynamic simulations of operations is sufficiently mature to enable the design of control strategy and controllers. The control design parameters have been developed in parallel. The control strategies and controllers designs can be verified in a closed loop simulation before being implemented in the field. Now, the change can be made from an heuristic design and empirical techniques to fundamental, model-based designs.

In the previous chapters the attention was drawn to process and equipment design. In this chapter, the emphasis is on hands-off operation of the process. It is not the intention here to elaborate on instrument or control design, but to make the reader aware of the opportunities to achieve the objective of hands-off operation. The realization of the design philosophies, “Design for total quality control and first pass prime operations”, forms the starting point for automation and control. The basic control system and instrumentation are the base for operation optimization (see **Chapter 9**), and site-wide and remote operations as reflected in the operational hierarchy (Figure 8.1). It is the combination of process design and control design which makes the concept of simple and robust process plants a reality.

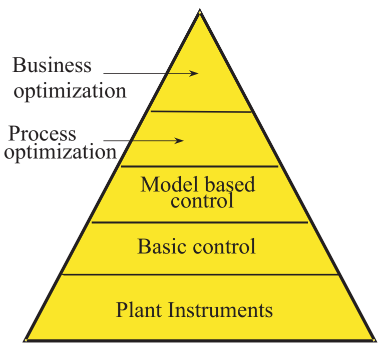

Fig. 8.1. Hierarchy in operation.

8.2 Instrumentation

8.2.1 Instruments

Instruments are the eyes, ears, and hands of the process. During the 1980s, the following striking points were identified:

- 50% of our instruments lie, or die
- Instruments during start-up and restart are unreliable
- Most process outages are caused by instrument nuisance.

It is clear that hands-off operation of a simple and robust designed process, cannot be achieved under these conditions. It was recognized that the above statements were an exaggeration of the situation, but the message was clear. The demand on instruments was increasing in order to achieve a high level of automation and control, on the route to hands-off operation. The causes of these bad experiences with instrument performance were multiple, and causes for instrument failures can be classified as:

- Instrument failure
- Selection of instruments
- Installation of instruments
- Interpretation of signals
- Maintenance of instruments

Although failures will always happen in these classes, it was the number of failures which needed to be severely reduced.

In order to obtain a more defined insight into the number and type of failures, these were monitored for several processes – batch as well as continuous. The instruments were monitored over a two-and-a-half-year period during the late 1990s. The instruments tracked were flow, level, pressure, temperature, and valves – these being the core of process plant operations. It should be noted that the measurements were installed during the 1970s and 1980s, and by far the majority were installed to monitor:

- Flow, orifices with a dP cell
- Level, dP cells with lead lines
- Pressure, transducer
- Temperature, a mixture of thermocouples and resistance temperature measurements (PT100)
- Valves, several types of block and control valves

A failure was registered every time an instrument technician was called for any supposed malfunction.

Table 8.1. Number and type of instrument failure in 2.5 years for different process measurements.

Type of measurement	***Flow***	***Level***	***Pressure***	***Temperature***	***Valves, including actuators and solenoids***
Type of failure					
Sensor	27	18	21	46	
Electric connection	9	6	8	50	
Electronics	21	5	14	0	
Electronics grounding	8	2	4	6	
Signal drift	28	30	13	3	
Accuracy	12	3	6	1	
Mechanical	44	30	8	9	
Lead line plugging	184	324	131	–	
Frost	3	6	3	–	
Instrumentation system Hardware	2	1	1	0	
Instrumentation system software	11	4	5	2	
Installation	8	3	8	3	
Process	21	14	24	4	
Other problems	34	101	33	27	
No problems	106	123	41	31	
Total failures	518	629	320	182	2121
Total measurements	873	923	1322	2302	13263
% failures/year	23.7	27.3	9.7	3.2	6.4
Failures leading to:					
Process disturbances	20	14	13	2	
Process trips	2	1	1	0	

The results are shown in Table 8.1, from which the following conclusions could be drawn:

- The percentage of instrument failures as experienced per year would be significant for an automated plant.
- The number of process disturbances and process trips are low in comparison to the number of instrument failures.
- The type and number of failures per measurement clearly identify the weak points
- For flow, level and pressure the top two failures are "lead lines" and the category "no problems"; these are responsible for over 50% of the reported failures.
- The "lead lines" are the top contributor.
- The "no problem" failures which are a fault diagnosis, mainly by operation are strange phenomena, but the ratio to total failures is between 12% and 20%.

- The two top contributors to failures for temperature measurements are the sensor and electrical connections; these are responsible for over 50% of the failures.
- For valves the percentage of failures in relation to the installed base was low compared to flow, level and pressure measurements. The type of failures are not available, but bad stem travelling and hysteresis are the most frequently observed phenomena.

These data provide a good indication of the reliability of instruments as designed during the 1970s and 1980s. Since that time, much effort has been spent (particularly by vendors) to improve the reliability of instrumentation. Progress made in this field is described below for the most commonly applied instrumentation (Liptak and Venczel, 1982).

8.2.2
Instrumentation Systems

Instrumentation systems have been through a complete development cycle. During the 1960s, single loop pneumatic controllers were standard, while off line computers were first used for engineering calculations and for some specific off-line operational models. The next step was the introduction of computers for steering sequential operations, all of which were based on digital actions. In particular, batch operations (and also regeneration operations) benefited from the consistency in automated operation, the result being improved quality and increased capacity.

Electronic single loop controllers were first introduced in the 1970s, at which time small-scale set points were regulated by a supervisory computer system. By the end of the 1970s, multi-loop computer-based control systems had been introduced for analog control, based on direct digital control (DDC) technology. Control systems were further developed in the 1980s and 1990s, when the combination of digital and analog operational functionality was realized. Subsequently, computer power was increased and screens were introduced as the operator interface to replace the large panels. More sophisticated control activities could be implemented in this system, which included model-based control. A computer system for intensive operational optimization calculations and set point steering was installed on a higher level of the control hierarchy. The hierarchy for control is shown schematically in Figure 8.2.

In the 1970s, the pneumatic signal transmission was to a four-wired electronic system, though this was later replaced by a two-wired system where the power for the instrument was combined with the signal. This was all based on analog signals.

The development of a so-called “fieldbus” – a core cable for digital data communication to replace all the individual wiring – occurred at the end of the 1990s, and was standardized in IEC 61158. The initial drive for this technology was cost reduction for wiring. The technique of digital data communication opened a new world in instrumental design.

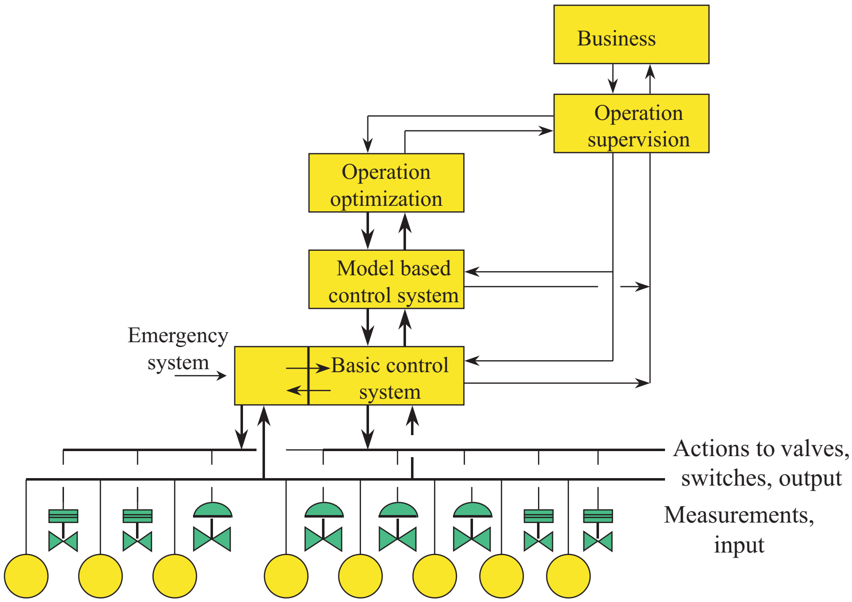

Fig. 8.2. Control structure.

8.2.3
Instrumentation Design

Instrument design was influenced by the introduction of micro-electronics using integrated circuits (ICs) also called chips. The application of these techniques at the instrument level led to the introduction of so-called "smart transmitters and instruments". These provided new means of increasing accuracy, applying fault detection and auto-check and robust instrument design resulting in improved instrument reliability. Accuracy was improved by the application of corrections for ambient temperature variations for the different type of measurements.

In combination with digital communication, signal analysis over a broad spectrum may be applied for the early detection of approaching undesirable process conditions. An example is the detection of pump or valve cavitation by signal analysis of pressure measurements located close to the device; alternatively, the effects of bad functioning control valves can be identified by flow or pressure analysis The specifics for the most common instruments are discussed in the following sections.

Flow measurements were – and still are – typically performed with a cheap orifice measurement provided with a dP cell. The element is reliable and robust, but it measures ρV^2 (ρ = density; V = velocity); hence, the measurement of flow is in units of neither mass nor volume. This can be seen as strange, since although the mass flow was required for an operation, we were satisfied with obtaining a value for ρV^2. Normally, mass flow is derived by calibration at a fixed density. The signal is wrongly interpreted, as density changes caused by temperature or concentration deviations are not recognized (except in commercial measurements where displacement measurements are installed that are generally corrected for temperature and density). Another problem is that, for correct installation, an installation length is required upstream and downstream of the meter, and this is seldom the case. In specific situations, temperature and density corrections are applied. Plugging of the lead lines is another frequent cause for failure (see Table 8.1). The design errors in this example are the selection of the instrument, the installation, and interpretation of the signal.

A robust, reliable solution is found in the application of Coriolis meters for mass flow; these are supplied in one embodiment with a density and temperature corrections. These type of measurements also avoid installation of the lead lines.

Level measurements are typically performed by dP cells. The measurement is effected by lead lines which are assumed to be filled with process liquid. During start-up, these lines are often not filled, and during operation the density of the liquid in the lines fluctuates with ambient temperature. Plugging of the lead lines is a frequent cause of failure, especially when water is trapped in the lead lines, this being a common cause of blocking during freezing weather. A more reliable solution is to use remote seals that avoid fouling and blockage, though the signal is then affected by thermal expansion. Level measurements on dP cells are increasingly replaced by capacity or ultrasonic measurements (as these are more reliable), or by subtraction of two independent pressure measurements.

Pressure measurements are typically membranes, where pressure was transformed into mechanical displacement that could be measured. In the past, this movement was provided by a mechanical pointer, while in the next generation the displacement was converted into a pneumatic signal available for pneumatic control. Clearly, it was possible to convert this device into an electronic unit; this improved the accuracy because the mechanical displacement required was reduced, and so in turn was the hysteresis of the membrane. Currently, the measurement of pressure is achieved using a piëzo crystal, which requires a minimum displacement and can resist pulsed pressure; this is altogether a more robust design. Installation is carried out at the vessel in order to avoid lead lines, the result being improved accuracy and much greater reliability.

Temperature measurements also underwent evolution, starting with mechanical displacement devices such as bimetallic or thermal expansion-based units. The thermocouple, using different types of material combinations, was a good successor in the electronic time-frame. For an adequate measurement, those materials were selected with a relatively high emf /°C, such as Fe-constantan. The cold junction of a thermocouple suffered from ambient temperature variations. The resistance thermometer partly replaced the thermocouple due to its greater accuracy, its disadvantage being that a three-wired system is required. In the digital age with completely sealed ICs being used for measurements, the thermocouple is again in focus. Cold junction temperature variations are compensated with the local IC, while the emf versus temperature curve is brought into the IC.

The selection of thermocouple materials is now driven by less corrosive materials such as Ni-CrNi, the emf generated dominating the selection to a lesser extent. The selection of these less corrosive materials and the improved sealing and compensation techniques make current thermocouple devices more accurate and reliable. Recall that the sensors and electronic connections were the major contributors to failures of temperature measurements (see Table 8.1).

Switches are candidates for frequent failures, while detection of failure is only experienced during testing. Failures are mostly caused by plugging. Switches on levels of vessels or pressure are replaced by installation of two parallel analog measurements provided with software switches. In case of an element failure, diagnostics of the analog signals can easily assign the failing element. In the past, frequent failing of switches installed on on–off valves to confirm the valve position was a nightmare for operation due to the high failure rates. A standard response was to ignore the signal, but this is unacceptable in a hands-off operated process. The solution came from the suppliers who currently deliver totally enclosed sets of switches based on the inductive principle. This replaced the mechanical switch which was less reliable for on–off valves, and avoided the impact of weather conditions. As a result, both the reliability and robustness of the design were significantly improved. The option to minimize switches on open and closed condition of block valves is still preferred for nonfouling and low-temperature applications.

Valves – particularly block valves – might be subject to sticking by fouling or any other cause, such as a malfunctioning solenoid. These valves currently will still need some attention from maintenance. Control valves in general have a low total failure rate, but are subject to wear that results in hysteresis and pulsed displacements. These problems need to be monitored, and signal analysis of flow or pressure measurements on the same line can identify this problem to be used for predictive maintenance. The selection of type and size of control valves deserve more attention to achieve good operational performance over its required operational range

Analysis and analyzers have been the subject of breathtaking development. During the 1960s, nearly all analysis were performed at the laboratory, using wet chemical analysis. This required samples to be taken by operators and delivered at the laboratory – this had already introduced errors. Next to its time-consuming analytical effort, this approach was subject to human errors and the low accuracy of analytical procedures. During the 1970s, automated physical laboratory measurements were introduced, such as gas chromatography (GC) and infra-red (IR) meters, while during the 1980s and 1990s the development and in-plant installation of process analyzers was a major factor. The analyzers went through a development cycle to improve the accuracy and reliability, and the interpretation of results was greatly improved by the installation of microprocessors. In particular, GC was handicapped by the batch analytical technique which required sample taking, handling, and injection of very small quantities (a few μ l), and this renders the system vulnerable to failures. In contrast, the large response time (which was a major handicap for control applications) was greatly reduced by the use of capillary columns rather than packed columns. The process analyzers were also provided with auto-check, auto calibrate functionality and fault diagnosis. Process analyzers achieved accuracy levels that were higher than the off-line analysis. The disadvantages of the analyzers were still the sample taking and handling, and the related long response times, and this forced development effort in the direction of in-situ (or in bypass loops) installed optical measurements including UV, IR, near IR (NIR) and Fourier transformed IR (FTIR).

A good example of this technique is flue gas analysis with IR. Sample taking was the main handicap of this application, the sample needing to be sucked from the stack. Condensation in the sample lines was problematic, and the response times were long. In-situ measurement overcame these handicaps. Only a few of the available techniques are mentioned, but the trend is towards greater accuracy and reliability, and shorter response times. Thus, these units can be included in a control loop.

Although the development of the most common measurement techniques have been discussed in the previous section, many more measurements have been subject to the same development cycle. The improvements made have addressed the major failures of instruments as detailed in Table 8.1. The improvements in the reliability of instruments are important for robust operation, as nuisance trips are often caused by instruments and also by "over-instrumentation". We mentioned earlier the objective of a two-engine airplane flying over the ocean at the same level of reliability as a four-engine counterpart. The same approach is applicable to instrumentation, and therefore process plants will benefit from more reliable, but fewer, instruments. Some data were collected for nuisance trips concerned with compressor trains. Four multi-stage centrifugal compressor trains with drivers of around 20 MW were monitored for 4 years during the late 1990s, the number of trips being totaled and categorized:

- Instrumentation
- Process
- Mechanical
- External cause

The results are shown in Table 8.2. Although the number of data are limited, it may still be concluded that the number of trips due to instrument failure are high in this data set (50%). The mechanical failure is a clearly identified other cause. The other "trips" were registered as process and externally caused trips, though the data did not indicate the original cause of these interruptions. These data illustrate the importance of the reliable instruments that are superseding mechanical failures, though it should be noted that instrumental trips (in general) result in short process stops. Mechanical failures might result in considerably longer outages. The failure rate data for the improved measurements as discussed above require collection, as these are needed for instrumental design.

Table 8.2. Causes of nuisance trips of four major multi-stage compressor trains (including the drivers) over a 4-year period.

	Instrumentation	***Process***	***Mechanical***	***Outside cause***
Number of trips	10	5	1	4

8.2.4
Safety Instrument Systems (SIS)

The design of safety instrument systems (SIS) is a way of improving the protection of process plants, and this approach has found a much wider application. The protection of an ammonia pressure storage tank was shown in Figure 3.5 in **Chapter 3**, where the design was simplified by the installation of SIS. Other, similar situations also exist, such as the early detection of a runaway reaction, where a SIS can protect the process by timely adequate instrumental actions. These situations are more difficult to handle by conventional hardware safety relief devices. At the moment, pressure relief devices detect the extent of the runaway reaction at such a point that large quantities of chemicals have to be released. These amount are difficult to recover, and might cause high environmental loads. Furnaces are also provided with burner management systems for protection against uncontrolled reactions such as explosions. The design and maintenance of these SIS are prescribed in IEC 61508, this approach being referred to as the "Life Cycle Safety". The SIS need to operate over the process lifetimes, and therefore include maintenance and inspection activities to keep the SIS up to date.

The first step of the quantitative methodology in the design of SIS systems consists of determination of the safety integrity level (SIL). The SIL is a measure for the risk of a process, the risk being impacted by the likelihood of the event, and the consequences. The consequences are divided into three terms: personal safety; production and equipment loss; and environment. In IEC 61508, the average probability of failure on demand (PFD_{AVG}) for protective systems of low demand has been defined and is given in Table 8.3.

The design of the SIS must meet the criteria of the applicable SIL. The design is a quantitative approach where not only PFD_{AVG} is calculated but also the number of expected false (nuisance) trips must be quantified. Several SIS configurations are evaluated at that stage. The SIS must be analyzed for reliability and availability for all components in the loop from sensor, transmitters, wiring, instrumentation system hardware as well as software, actuators as switch, final element, power supply, air supply, response time, maintenance and operational procedures. For the SIS alternatives, quantitative fault trees are developed to determine the average PFD and nuisance trips. A common mode failure needs to be part of the analysis. The optimal

Table 8.3. Safety integrity level and the average probability of failure on demand for a low-demand situation (IEC 61508).

Safety integrity level	*Average probability on demand*
4	$10^{-5} < 10^{-4}$
3	$10^{-4} < 10^{-3}$
2	$10^{-3} < 10^{-2}$
1	$10^{-2} < 10^{-1}$

SIS must be selected based on PFD requirements. The development of a reliability database, particularly for the recently developed instrumentation, is a priority to enable the design of simple SIS.

8.2.4.1 **Design guides**

Instrumentation plays a major role in the design of simple and robust plants. High instrumentation reliability and availability are major objectives to achieve simplicity (less redundancy in instrumentation) for operation. Instrumentation is a term in the complexity formulae (see Section 2.2), which includes the point that reduction of instrumentation reduces complexity. Numbers of nuisance trips which are not really appreciated by operation will also be reduced by more reliable and less superfluous instrumentation. It is instrument unreliability that is the source behind the demand for instrument redundancy leading to nuisance trips. Robust process control will more than benefit from good instruments, and is a precondition for hands-off operation and control.

For instrumentation of simple and robust process plants several design guidelines were outlined in Section 5.7.4 in **Chapter 5** These design guidelines are rephrased and completed in the following points:

- Apply only reliable and robust instruments, and let these measure what you want to measure. Most of the time we like to measure and control mass flows. Traditionally, this was done by measuring volume, which only in exceptional cases was corrected for temperature and density changes.
- Develop good instrument selection and installation procedures that ensure instruments do not have to “lie or die” and are available and in good condition during start-up.
- Apply instrument fault detection
- Apply preferable instruments with sensors in process lines or in slip streams (long sample lines cause delay times).
- Avoid lead lines for pressure transducers and level measurements as they are a source of failures.
- Avoid batch-operated analysis like GC if alternatives are available. GC is accurate, but requires sample handling and injection systems. Sample handling and the analysis have long response times, while injection systems are sensitive to fouling.
- Apply single instruments with fault detection, and deviate only in case of safeguarding with SIS. Experience has taught that double instruments are a nightmare for operation as they cannot easily decide which one is wrong. An exception might be made for batch processes where accurate dosing of components that determines product quality and safe operation conditions are a firm requirement. An accuracy check is mostly done by load cells installed on process vessels.
- Avoid local instruments. Simple and robust process plants do not have field operators to watch the process outside – it is monitored from the control room.

- Control valves need to be adequately sized (do not oversize), and manual bypasses are to be avoided. Control valves are very reliable, but we should not operate without them as this will lead to uncontrolled situations.
- Switches on block valves are advised for fouling or higher temperature systems, where the likelihood of sticking valves is relative high. For emergency block valves these are advised only on the failsafe position.
- Diagnose instrument signals by spectrum analysis to detect/alarm operational or mechanical problems. Instrument fieldbus or other digital communication systems makes this a possibility.

Simplification finds it way in the above guidelines by single reliable and robust instruments, which are properly selected, installed, operated and provided with auto-check.

8.3
Automation of Operation

Automation takes care of implementing the operation strategy which plays an important role in simple and robust design concept (CCPS, 1993; Rijnsdorp 1991). As "Why automation?" is a legitimate question to ask, we have to look at the characteristics of human beings as mentioned earlier (**Chapter 3**) under the design philosophy: minimize human intervention (CCPS, 1996).

One of the main human characteristics which justifies it is:

Human beings cannot consistently perform tasks.

Each time that people need to repeat certain activities, they will perform the task – but always with some interpretation of the way this task can be completed. They will not react timely and follow different sequences, but are also handicapped by human errors. In the process industry it is necessary to make products of consistent quality with a minimum of variation, and such an objective can only be met by automated processing and hands-off operation. Safety systems are designed hands-off based on the same reasoning.

Another quality of character is that:

If it is to complicated, no one will be able to figure it out.

When something is difficult to understand or is complex, people will either not touch it, or will switch it off. In the discussion on simplicity and complexity (**Chapter 2**) it was said that complex operations require total automation. A model-based controlled or an operation optimization-controlled process is an example of where the design of these controllers require a high level of robustness and availability. If these requirements are not met, they will be "switched off" by operation. Complex operations demand for total automation.

A character trait of human beings is also their limited memory or even wrong memories, phrased here as:

If you don't have to memorize, you can't forget it.

Automation solves this problem. The computerized systems can recall instructions and procedures exactly over its lifetime. To accommodate this loss in memory, operational software can easily be provided with status overview and progress in operation sequences and terms and conditions to be fulfilled for transient operations.

Automation always triggers the question, "How far do we automate?" Quality and economic requirements drive us to more consistent production with less variability, while production is optimized. The operation of simple and robust plants will be grouped more and more in one control room. The approach of simple and robust is full automation, but there can be some economic constraints to this approach. It should be noted that simple and robust might lead to some more process trips. Due to full automation and fewer operational personnel, the process will trip more in situations of failures or supposed failures, which in the past was how the process was kept "on air" by operators. The automation of all activities that require frequent operational activities are beyond the discussion here. All batch operations are automated like batch reactors, batch extraction but also regeneration for adsorption and de-sorption units, reactors. The start-up of a unit might also lead to a dangerous situation if not automated like furnaces that require a burner management system for start-up.

Also interlocking and process trips require automation as the operation crew is not available nor consistent enough for manual operation. The debate starts about the start-up of continuous processes which have very long production times without interruptions. The latest world-scale ammonia plants have experienced uninterrupted production of 4 years, and clearly in such cases a complete automated start-up might be costly. In those specific cases one might develop a start-up procedure that should be loaded in the instrumentation system and tracks and verifies the start-up by the system, in case a start-up team is required (Stassen et al., 1993; Wei Zhi-Gang et al., 1998).

8.3.1 Instrumentation Selection (Analog In and Outputs and Digital In and Outputs)

The bases for the instrumentation are the operational and control strategies. The instrumentation selection is performed from different viewpoints:

- Control, CVs and MVs (controlled and manipulated variables)
- Automation of operation (digital actions and operational trajectories)
- Safeguarding
- Observation, including performance measurement

The most common type of measurements are:

- Flow
- Pressure
- Temperature
- Level/ height/weight
- Speed
- Vibration
- Position
- Physical properties like; density, viscosity, color
- Components such as O_2, CO, gas detection
- Composition

For *control*, the required selection of instrumentation of the process is mostly foreseen at its steady-state or quasi steady-state conditions based on a designed control strategy. These are mainly the CVs and MVs, reflected in the AIs and AOs, the selection of which is discussed under control design, (see Section 8.4).

8.3.2
Automation of Operation Based on an Operational Strategy

The basic question is "how to operate" the process, and the answer to this forms the basis for the operational procedures and the related software.

The objective is the *controlled start up, shut down* and any other *operational transients* of a process plant along a defined pass way *not violating any of the unit and process constraints.*

For the operational strategy of a simple and robust process plant, the emphasis must be placed on a few points regarding its implementation. It was concluded earlier that the drive is for total automation. It has also to be understood that, under normal circumstances, operation is not "available" for direct manipulations (operating valves) and are not to be seen as part of a control loop.

The drive remains for TQC. This is not restricted to the full operational state (also called the "run state"), and the challenge is to produce a prime product from the start – this is called *First pass prime production* (FPPP).

This opportunity has been proposed in **Chapter 3** as a challenge to remove or minimize all process equipment and logistic needs required to deal with off-specification production. An overall operational strategy needs to be designed for process operation, and is described below based on the work of Aelion and Powers (1991) and Verwijs et al. (1995).

The operational strategy is a systematic approach which designed heuristically, and contains the following elements:

- A set of operational objectives which are:
  - safe and environmental sound production,
  - total quality control (TQC) with first pass prime production (FPPP) and just in time production (JIP)

– total automation
- A layered structure of operational states which have to be passed in defined sequential order
- Defined transient operations to bring the process from one operational state to the next.
- A set of detailed operational procedures

The operational states of a process are defined in the area from start until full operation at required specification. The full operational state for a continuous process – the "run state" – has an operational range. There can be several intermediate states defined for a process, ranging between no operation and full operation. An example of a process with four operational states is shown in Figure 8.3, from a maintenance state through a process wait state with utilities available and the system filled with process material, followed by a process state with internal reversible operation systems active up to the run state the highest operational state. On this graph the transient operations are visualized by vertical arrows. Upward-pointing arrows reflect the start up transient operations, while downward arrows represent transient operations to bring the process in a controlled manner to a lower operational state. The dotted arrows represent the interlocking or trip actions which bring the process or part of the process abruptly to a lower defined operational state. A process is divided into different sections or units, all of which have defined operational states that are a subset of the overall process state.

Each operational state is defined and has its specific operational targets with a defined range and constraints applicable for units, sections, and the overall process.

- The defined targets with its ranges are reflected in process conditions such as flows, pressures, temperatures, qualities, levels, and speed.
- The defined constraints are set by product quality, safety and environment.

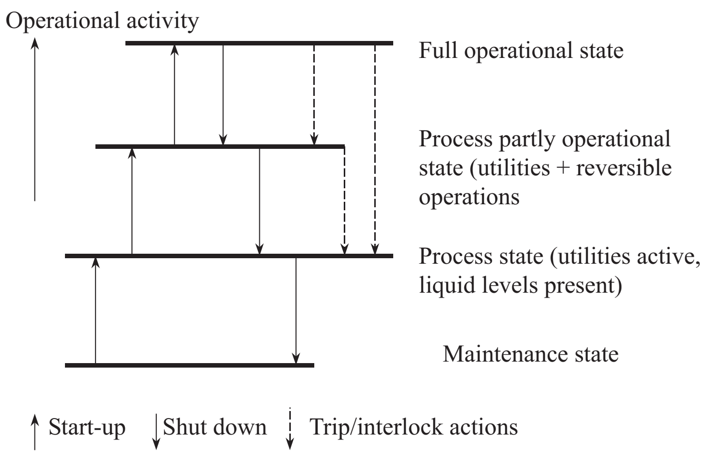

Fig. 8.3. Operational states from full run state still no operation.

The selection of specifically the intermediate states of the units/sections should fit in a start-up/shut down sequence of the overall process. In the process plant, units (or combinations of units) can be identified which can run independently from overall processing. The presence of simultaneous inverse operations within system boundaries makes it possible to create a stationary state, like heating versus cooling and separation and re-mixing (Fusillo and Powers, 1987, 1988). Examples include a refrigeration unit which has an evaporator and a condenser in the unit, and a distillation column operating at total reflux. It was Verwijs et al. (1995) who introduced the terms "reversible" and "irreversible" unit operations.

A *reversible unit operation* is defined as "... a process system that can be operated stand alone, without any process streams fed into or exiting subsystem due to the presence of inverse operation". This opens the possibility of conditioning a process system during start-up. Conditioning in this aspect should be understood as bringing the process system or unit close to its planned operational conditions to accommodate a controlled start-up. As a pre-requisite, Verwijs et al. (1996) mentioned the simultaneous operation of the inverse process functions which can be achieved by recycling material. An example to be mentioned here is a distillation column where the top and bottom products are recycled to the feed, while there is no fresh feed. Another example is an absorber–stripper combination where the solvent is recycled over the absorber and stripper with its heaters and coolers active, while there is no feed stream fed to this section. A reactor system for an equilibrium reaction can often be operated as a reversible unit by recycling the outlet streams.

Irreversible unit operations are started up by adding feed into the system, whereupon the unit has to start. An example of such a unit is an irreversible reaction system as shown by Verwijs et al. (1992) in an overall flowsheet for an exothermal hydration reaction (Figure 8.4). Other examples of irreversible operations next to irreversible reactions are drying filtering.

By distinguishing between reversible and irreversible units operations, a guide can be made for planning the sequential order to start a process plant. Reversible units are put into operation first.

Before the overall sequential order for start-up/stop of a process is discussed, the start of a reversible and irreversible unit operations are discussed.

8.3.2.1 **Start-up of a reversible unit operation**

The reversible unit selected is a distillation column of which start-up is described step-wise.

1. Fill the distillation unit with normal feed from the feed point.
2. Take the top condenser in operation and put the reflux level loop in operation (total reflux situation).
3. Start the reboiler and build up the level in the reflux drum at the expense of level in the bottom. The loss of level in the bottom is compensated by adding some more feed.
4. Bring the unit to its operational conditions with at least one product stream (preferably the most critical) at its required quality.

5. Start recycling the top and bottom streams to the feed vessel while feeding continuously from the feed vessel and bringing the distillation column at its operational conditions including both product qualities.
6. Reduce the recycle and gradually bring fresh feed to the required amount.

A breakdown of operation in its functional activities is: first, the system is filled; second, the unit is brought at operational conditions, heat addition, pressure and inventory control with flow and level loops active; third, qualities are in control; and fourth, the unit is brought to full operation.

Alternative ways to start such a system include filling the reflux drum and bottom section with material at or close to specification, in which case the column can be brought more rapidly to its required operational conditions. Another option is to recycle the product stream immediately to the feed vessel before the products are at quality. Whichever route is used, the objective is the same – to bring the unit operation to its operational conditions that enable smooth processing of freshly supplied feed at any time, by achieving inventory control and simultaneous heat and mass balance control (all control loops are now active).

The advantages are that the unit is available for processing, and the impact of upset on successive unit operations is limited.

8.3.2.2 Start-up of an irreversible unit operation

Irreversible unit operation demands another approach in order to realize first-pass prime operation, for which two options are available:

1. To determine if the unit operation can be made reversible by implementing an inverse operation. For example, a crystallizer can be made reversible by dissolving the crystals formed and recycling them back into the feed.
2. To accommodate the operational conditions of the unit in such a way that when the feed starts it can perform its function. Start-up of a dryer is mainly done by preheating the dryer beforehand to the required level; in this way a dry product is obtained immediately after the feed is processed.

A start-up approach was generated for an irreversible reaction and studied by Verwijs et al. (1996) for the process shown in a simplified form in Figure 8.4. This study is summarized below to illustrate the possibilities for the start-up to meet first-pass prime conditions. The reaction studied was an irreversible, noncatalytic exothermic hydration reaction, and is described as

$$A + B \rightarrow C$$

Some consecutive reactions take place which were not relevant for this study.

The reaction is adiabatic and performed in a plug flow reactor, all in the liquid phase. The reaction was first-order, with an Arrhenius-type rate equation. Reactant A is in excess, and therefore after separation from the reactor effluent is recycled back to the inlet of the reactor. The objective was to achieve a high level of conversion for reactant B in order to avoid the formation of an undesirable reaction after the reactor. This condition is particularly important during start-up as, during this

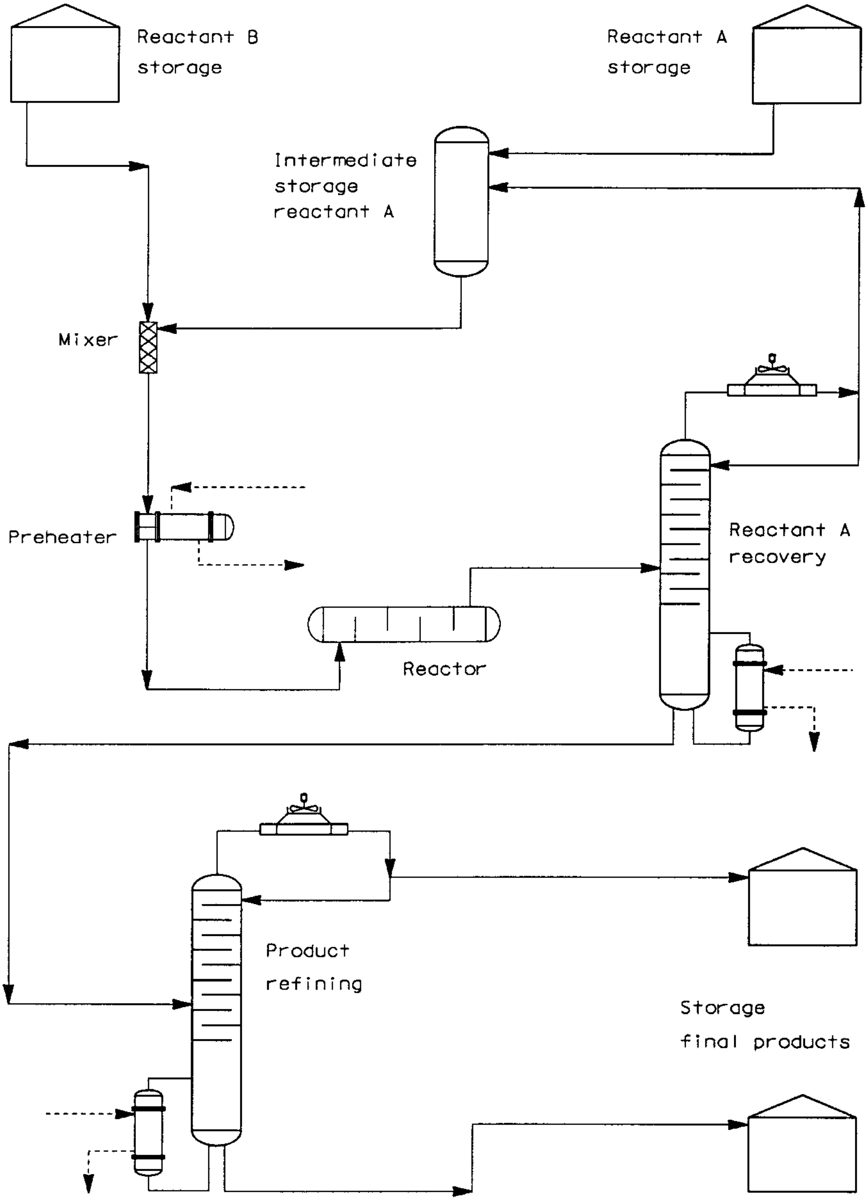

Fig. 8.4. Process scheme of a continuous process for operational studies (Ref. Verwijs '95 AIChE).

transient operation, the likelihood of a breakthrough of component B is high unless specific precautions are taken. This system was studied through dynamic simulations and optimizations to search for operational transient conditions under which FPPP could be realized. In this particular example, FPPP was defined as staying below a certain specified level of component B in the reactor outlet during start-up.

The controlled variables (CVs) are:

- Mass flows of A and B, and through them, the production rate.
- Reactor inlet temperature.
- Outlet concentration of component B.

The manipulated variables (MVs) for the reactor are:

- Reactant mass flow B is controlled by a control valve in the feed line before reactant A is added.
- Reactant mass flow A is controlled indirectly by manipulating the total reactor outlet flow.
- Reactor inlet temperature is controlled by the manipulating the heat flow to the reactor pre-heater.
- The manipulation of the trajectories of the three MVs over time.

For observation and safeguarding temperature measurements were installed over the length of the reactor. For the study of the reactor start-up, a dynamic model reactor model was developed by describing the main reaction, this for reasons of simplification.

A reactor start-up strategy was developed in four consecutive steps to start the reactor up and to attain full operational conditions:

1. The reactant A is recycled over the entire process section, which includes part of the recovery section.
2. The recovery section for component A is brought to operational conditions.
3. Reactor inlet temperature is driven to operational conditions θ (z, 0) at which reactant B can be fed safely in the reactor.
4. Supply of reactant B to start production. The condition achieved at the end of step 3 is the state of the reactor at time 0.

For the start-up, the degrees of freedom explored within the operational strategy are:

- Initial reactor inlet temperature at the introduction of reactant B.
- The total reactor flow rate ϕ_i for start-up.
- The flow rate trajectory of reactant B.
- The trajectory of reactor inlet temperature $\nu_{\theta,}$ with as initial condition is θ (z,o), and the normal operating condition θ (o, σ).

The final reactor conditions at full operation are known from steady-state simulations.

The system was described in dimensionless terms by using a reference value, the symbols used being:

- z is axial reactor position
- α_1 decrease rate parameter for reactor inlet temperature
- α_2 increase parameter for flow rate
- ϕ_i is total reactor flow rate
- Γ_B is concentration of reactant B
- ψ_B is concentration of reactant B at the reactor inlet
- ν_θ is the trajectory of the inlet temperature over time
- σ is time
- θ is temperature

The manipulated variables over time are shown in Figure 8.5, the initial temperature having been chosen to be higher than the normal operating temperature. In the earlier studies of Verwijs et al. (1992) it was shown qualitatively that for an adiabatic tubular reactor a initial higher inlet temperature is required to ensure that no excessive amounts of reactant appeared in the reactor effluent.

The ramp functions of the reactant's flow rate and reactor inlet temperature α are linearized to make the optimization problem much simpler to handle. Minimization of the reactant B breakthrough value was selected as the objective function, while the constraints defined were:

- the maximum allowable operating temperature of the reactor;
- reactor flow;
- inlet temperature; and
- ramp-up rates of temperature and reactant.

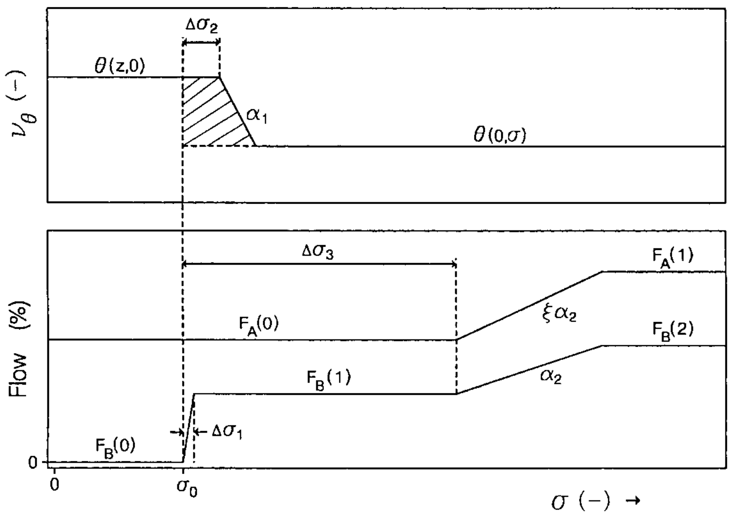

Fig. 8.5. Manipulated variables during reactor startup (Ref. Verwijs '95 AIChE) dimensionless factors: σ is time, θ is temperature, α ramp up/down rate, F is flow.

The trajectories of the manipulated variables ν_θ, ψ_B and φ_v and the inlet temperature are subject to evaluation, and the objective function is minimized by manipulating these variables.

The results were shown in three-dimensional graphs (Figures 8.6 and 7); the temperature and concentration profiles are shown as a function of reactor location and time for specified conditions. This example was chosen as it clearly demonstrates that reactor start-up can be achieved without breakthrough of a component. The same reaction system was also analyzed for the effect of process shut-downs and interruptions (see Section 8.3.3, Instrumental safeguarding). The overall flowsheet of the hydration process is shown in Figure 8.8.

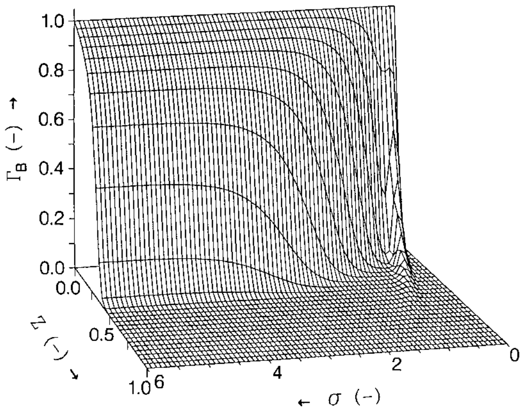

Fig. 8.6. Calculated reactor concentration profiles versus reactor location and time, (Ref. Verwijs '96 AIChE) dimensionless factors: σ is time, **z** is axial reactor position, Γ_B is concentration of reactant B.

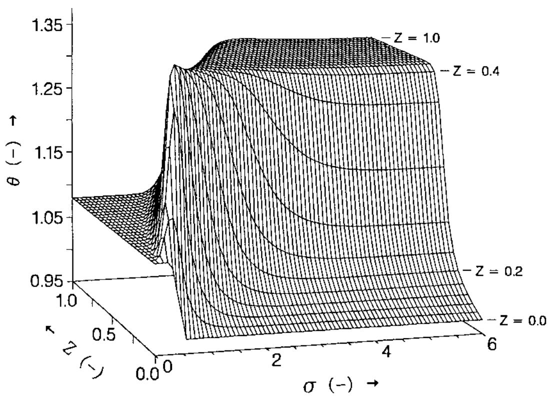

Fig. 8.7. Calculated reactor temperature profiles versus reactor location and time (Ref. Verwijs '96 AIChE) dimensionless factors: σ is time, **z** is axial reactor position, θ is temperature.

Similar dynamic simulations and optimizations can be performed for other irreversible reactor systems with defined objective functions. As example is the hydro-dealkylation (HDA) process where toluene is converted to benzene in a reactor system with a large hydrogen recycle (Figure 8.9). Benzene is the product, and diphenyl the by-product, this being a non-catalytic exothermal gas-phase reaction performed with excess hydrogen, and the kinetics and rate equations being well-known. A problem-free start-up, first-pass prime production of such a reactor system can be designed through dynamic simulations. There should be no reason why catalytic fixed-bed reactors (eventually cooled) or CSTRs could not be analyzed in a similar manner.

This technique proves that first-pass prime operation is achievable for irreversible plug flow reactor systems when a recycle is available to condition the system beforehand. A precondition for development of the operational strategy is that the main reaction kinetics and rate functions are known, although these need not be highly detailed for operational studies. However, the overall conversion rate must be described accurately.

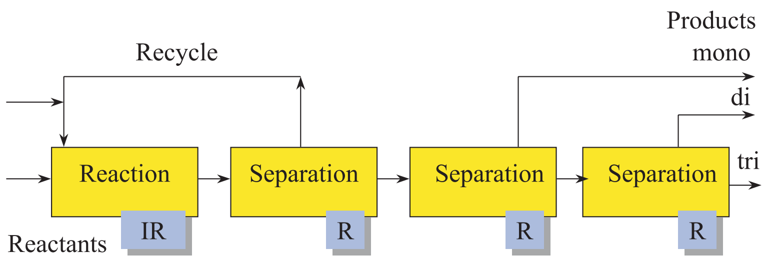

Fig. 8.8. Hydration process with irreversible reactor and reversible separations.

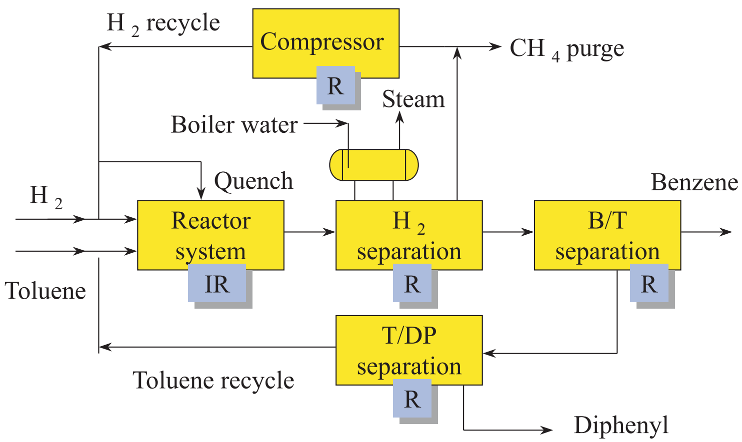

Fig. 8.9. Hydro de-alkylation process with irreversible reactor, reversible separation and compressor units.

Stoichiometric reactor systems at high conversion without a recycle for preconditioning are more difficult to design for first-pass prime. An example is a furnace, but this can be made reversible by installing a recycle or dummy load on the process side. On occasion, the flow of inert material takes the role of conditioning. An example is the nitric acid plant, which is shown schematically in Figure 8.10.

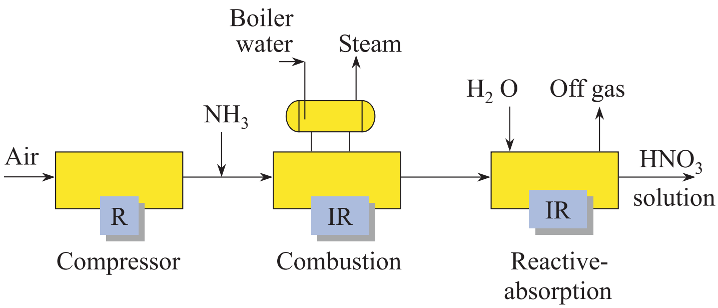

Fig. 8.10. Nitric acid process in a block diagram with reversible compressor and irreversible reactor and reactive absorber.

The nitric acid plant consists of three sections: an air compressor; a NH_3 combustor where nitrous vapors are formed and the exothermal heat is removed; and finally absorption in water to form the acid. In such a plant the nitrous vapors are formed by combustion of NH_3 with air; this reaction is almost instantaneous. An absorber column where these nitrous vapors react in water requires careful design for its operation. This process can be conditioned by the air compressor which passes through the whole process – in essence it is an open recycle system. To achieve the required acid concentration the water flow needs to be controlled for steady-state conditions. This is quite straightforward: during start-up the achievement of first-pass prime requires careful design of the operation, based on dynamic simulation. The control of a recycle over part of the column for start-up is a precondition.

Transient operations in continuous processes to achieve different product properties will always produce intermediate products, as in the case of polymer processing for polystyrene and polyethylene. One reason for this is that these processing systems mainly have a large residence time distribution, which results in a large transition zone that is inherent to the process design, another reason is trajectory control. Dynamic optimization of the transient operations can reduce the transition zone in as much as it is impacted by control. The dynamic optimization technique has now been developed and is approaching commercial status.

For batch processes, the production of first-pass prime products depends both on accurate metering of the feed streams and temperature control. Currently, the metering techniques are highly accurate, especially as redundancy is foreseen for dosing of mass streams by weight cells on process vessels. The argument for this is safety, but mass flows are also verified. The model predictive control techniques for batch processes are matured to achieve consistent temperature control. The higher consistency in mass flow and temperature control results in consistent batches. The objective for a batch plant to produce each batch at specification can be achieved with current techniques.

The conditioning of a process is not only limited to achieve FPPP but also to satisfy mechanical constraints. Mechanical systems are constrained by their capability of handling temperature transients. These constraints are respected by smooth start-up of units exposed to temperature transients. Units operated at extreme high or low temperatures may be fitted with temperature sensors for monitoring heating and cooling effects.

The smooth start-up of equipment subject to temperature transients is carried out manually, by slowly opening valves. If it is necessary for this to be automated through temperature trajectory control, then specific precautions must be taken for sufficient instrumentation with adequate valve sizing and selection.

The above discussion teaches us that FPPP, in most situations, can be achieved by careful process and operational designs. Dynamic simulation and optimization techniques for the start-up of irreversible reactions are efficient tools to design efficiently transient operations.

8.3.2.3 Start-up and shut-down of a process

In the previous section, three basic flowsheets of continuous process plants were described: a hydration process; a hydro-dealkylation process for benzene production; and a nitric acid process (Figures 8.8–8.10), all of which have different reversible and irreversible units. Here, the methodology is presented on how to start a continuous process plant, the three processes presented being those used for verification.

The methodology for **start-up** of a continuous process plant with a reaction and finishing section is:

- Take internal utility systems in operation which are in connection with external supplies, such as the power, steam grids, air, nitrogen and water systems.
- Take internal utility systems in operation not directly supplied from external, such as the process cooling water system.
- Fill and bring reversible process and utility units at an initial state called "process wait", such as filling up refrigeration systems with refrigerant, or filling process steam systems with boiler water.
- Take reversible utility systems in operation, such as refrigeration. For a refrigeration unit, partial heat removal is required, and this can be accomplished by lining-up a reversible process unit. (This reversible process unit must be brought to an initial state to remove any heat from the refrigeration unit.) The pressure and temperature levels of the utility systems are brought to (or close to) the objected operational conditions. The units will still operate at reduced loads due to lack of demand.
- Take reversible process systems in the operation, such as distillation, absorber-stripper or extraction-stripper combinations, by circulation.

- Condition irreversible process units close to operational conditions; this is often realized by setting up a recycle system or a dummy load, as applied for furnaces.
- Take irreversible process systems in operation to achieve quality product from the start by designed trajectory control.

When this procedure is applied, the three processes referred to during the previous start-up discussion of these plants are as follows:

- For the hydration process (Figure 8.8), the start-up takes the following sequential steps:
  - The utility systems are activated.
  - The last two reversible separations are taken in operation in reversible mode.
  - The reversible separation after the reactor section is activated.
  - The irreversible reactor is conditioned by putting the recycle from the separation as being one of the reactants, back to the reactor. Bring the reactor at start-up conditions with respect to temperature and pressure through a recycle.
  - Start the reactor according to designed trajectories for reactants flow and temperature.
- For the HDA process (Figure 8.9), start-up takes the following sequential steps:
  - The utility system are activated
  - The boiler is filled with boiler water and pressurized from the steam grid; the boiler unit is now at standby conditions. Strictly speaking, this is not a reversible unit at this point in time – it is only conditioned. It enters a reversible mode when the recycle compressor loop is active with the heater.
  - The reversible separations B/T and T/DP at the back end of the process are taken in operation.
  - The reversible compressor unit is put in re-circulation mode, together with the H_2 and CH_4 separations.
  - The initial heat source in the reactor system (an irreversible furnace operation) is activated; this is required to initiate the reactions. The boiler starts to produce steam, while the reactor system with its heat train is now conditioning up to its operational level.
  - Start-up of the reactor system with feed-through implementation of the designed trajectories for flow rates, temperatures and with H_2 quench.
- The start-up of the nitric acid plant (Figure 8.10) has the following sequence:
  - The utility systems are activated.
  - Accommodation of the steam reboiler by filling it with boiler water and pressurizing with steam from the grid (conditioning).
  - Fill the absorber with an initial amount of water; the trays are equipped with bubble caps with a high weir height to create sufficient residence time for reaction. A recycle over the bottom part. with acid is provided.
  - Start-up of the air compressor in open recycle mode over the atmosphere while bringing the combustor and the reactive absorber to open recycle condition.

– Start-up of the combustor is simultaneous with a programmed start-up of the absorber. The start of the absorber is dependent on the initial condition of the absorber, which often has an acid profile over the column at start-up, as the trays are full due to the high weirs and type of trays selected (bubble caps with cooling spirals for removal of absorption heat).

These examples illustrate the usefulness of the start-up methodology.

The **shut-down** of a process is preferably performed under *controlled conditions*. The shutdown is planned in such a way that the process and its units are placed in a defined safe state (intermediate or process wait), so that continuation of production or any planned maintenance can easily proceed. Selection of the specific intermediate state might depend on the time for which the process is projected to remain in that state. *Controlled conditions* refers to the operational sequence, as well as the time trajectories required to avoid any mechanical damage, for example causing too-great a temperature transient. The shut-down passways require careful examination, and are mostly performed in a reverse order of the start-up of the (ir)reversible units. Procedures may include specific steps, such as washing, steaming, and purging.

The operational strategy needs to be translated into a breakdown of all manipulations required for the operation of each unit. This results in the identification of automatic valves and motor switches with their DOs, in addition to the AIs and AOs which were determined during analysis of the control needs. Due to the unreliability of switches that come in contact with process fluids, these are only applied in exceptional cases.

Any additional instruments that are required to achieve first-pass prime operation should be added at this stage. These include the additional instruments required for batch reactions to verify feed quantities for reasons of product consistency. The total operational procedures must be written as a basis for operational software development.

8.3.3
Instrumental Safeguarding

Instrumental protection, including interlocking to prevent injuries to people, environmental loads and property loss, is detailed in this paragraph. Safeguarding is based on the following philosophies:

- Prevent a potential problem by eliminating or minimizing the hazard.
- Prevent loss of containment by equipment failure.
- Prevent the release of hazardous chemicals.

A protection philosophy was described by CCPS which is broadly used in industry and is based on:

- Building different protection layers (Figure 8.11) (CCPS, 1993).
- Design inherently safer chemical processes, with the keywords: Minimize, Substitute, Moderate, and Simplify (CCPS, 1993, 1996).

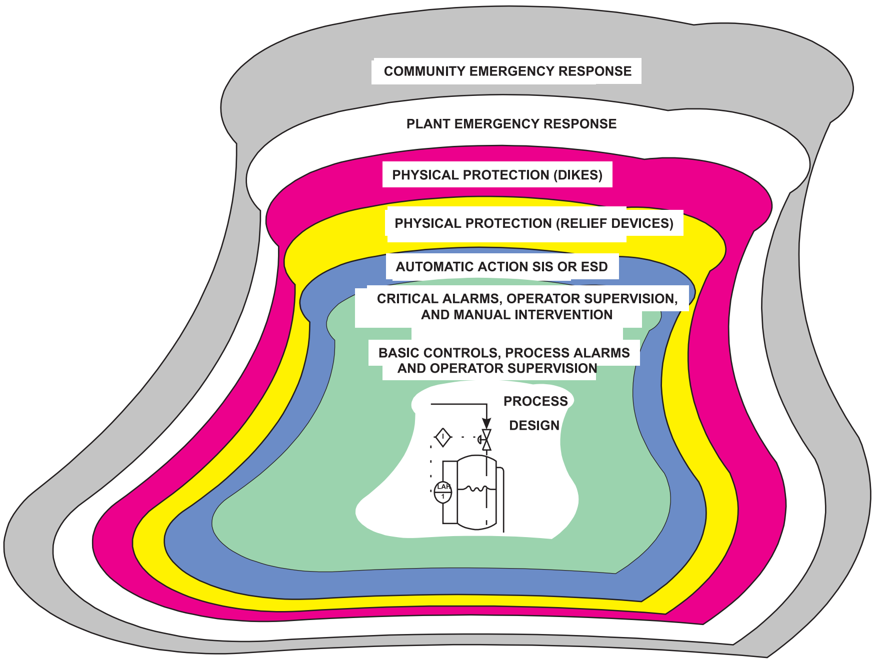

Fig. 8.11. Layers of protection in a chemical plant (Ref. CCPS '93 AIChE).

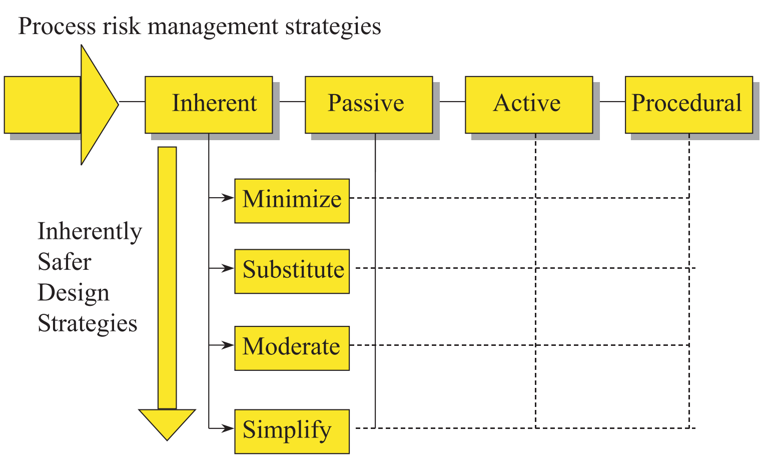

Fig. 8.12. Relation of process risk management strategies versus the inherently safer design strategies (Ref. CCPS '96 AIChE).

Specifically, CCPS (1996) is approaching inherently safer design which should be considered as part of this book. The strategy for process risk management in relation to inherently safer design is reflected in Figure 8.12 (CCPS, 1996). The illustration shows a decreasing reliability for process risk management in sequential order: inherent; passive; active; and procedural. The inherently safer design strategies are projected over the process risk strategies. The inherently safer design strategies are ordered as: minimize; substitute; moderate; and simplify, and are applicable for each process risk in management strategy. The approach reflects that for all safety protection layers – that inherently safer considerations are required. For the instrumental protection of a process, the plant concentrates on:

- Preventing loss of containment by equipment failure.
- Preventing the release of hazardous materials by a single instrument failure.

To achieve this, the different protection levels for the process are:

– Process design (eliminate/minimize the hazard).
– Basic control, including process pre-alarms (control the process).
– Critical alarms (warning operation for an approaching unsafe situation, where immediate action is required).
– Automated action, SIS (interlocking) or ESD (emergency shut-down).
– Physical protection (relief devices).

These represent the process protection layers that are directly connected to the process; all other measures are external provisions to reduce the effect of an event.

The instrumental and physical protection level ranges are shown in reference to the operating range (Figure 8.13). The safeguarding of a process plant depends for a large part on instrumentation, as the attempt is made to avoid activation of physical protection devices for hazardous releases. Activation of these devices often causes leakage of relief devices or mechanical damage, for example rupture discs and safety or crush pins. Rupture disks are not preferred as any subsequent release is much greater than would be, for instance, with a spring-loaded relief device.
In principle, the philosophy of inherently safer design starts with the elimination or minimization of the hazard, and this is especially applicable to simple and robust process plants. If this situation has been passed, protection should start at the point of initiation. The basic approach should be driven by the principle of:

Prevent versus cure

In order to determine instrumentation selection, all process equipment must be evaluated systematically, unit by unit, with the potential of exceeding design values for: pressure, temperature, overfill, speed, and vibration. Each time a need for a protection element is determined, the standard question should be: “can this situation be prevented?” This is fully in line with the inherently safer design principles. It is essential to follow this approach, and any prevention may include hardware modifications to the process. The prevention of releases and the related design of the SIS with interlocking needs to be based on the appropriate SIL level, all in line with IEC 61508 (see Section 8.2.4).

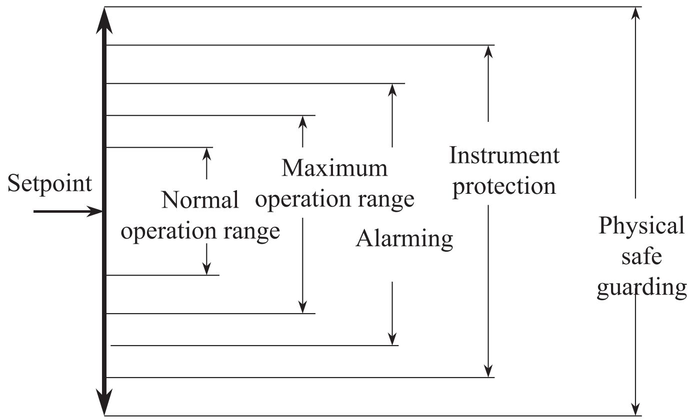

Fig. 8.13. Operating ranges with its protection levels.

At a later stage in the project, the piping and instrumentation are verified by HAZOP studies, to detect any remaining potential hazardous situation. Note that, during these evaluations, the target should remain: "Prevent versus cure". However, an additional design rule to be introduced here is:

Prevent the release of hazardous materials by a single measurement failure.

This rule is introduced because simple and robust plants with hands-off operation have limited numbers of operating staff who are able to detect or analyze specific situations. The consequence of the approach is that, next to the measurement for control purposes, a second measurement is present for potential hazardous releases, and this can be used for a higher level of alarming and interlocking. For systems which do not relieve outside the process, the measurement used for control can be provided with software switching for pre-alarming.

Reactive systems require particular attention as they might cause a run-away situation, with energy and gas release, specifically during transient operations. These situations must be prevented, and so call for early detection. When a pressure increase is noted, the temperature may already have been increased locally, and the reaction rates that are exponential with respect to temperature are already high. This often results in the relief of a large amount of energy and vapor/gas. This situation must be detected – and prevented – at an early point in its evaluation.

Verwijs et al. (1996) formulated this for an adiabatic plug flow reactor as:
"The spatial distributed nature and the transient behavior of the temperature readings along the reactor makes it significantly more complicated for operating personnel, in comparison with reactor safeguarding at steady state conditions:

- to identify important process deviations during dynamic operations;
- to recognize when a process is running into hazardous situations".

The same applies for batch or semi-batch exothermal or gas-releasing reactions, where a delayed reaction may happen that results in the build up of too-high concentrations of reactant. Subsequently, this situation may cause too-high reaction rates later in the batch, resulting in an uncontrolled run away reaction.

These situations need adequate protection. For the adiabatic plug flow reactor the system can be safeguarded by running a computer model of the reaction in parallel to the actual reaction, and using built-in deviation settings for alarming and interlocking. An alternative for real-time running of the model is to compare the reaction with historic reaction profiles of the planned transient operation.

For batch reactions that are normally operated at isothermal conditions, the above method requires another approach. In that case, a cumulative heat balance can be measured around the reactor. This is used to calculate the conversion of the reactants, by comparing this with the cumulative reactant feed times the heat of reaction. The amount of unconverted reactant can be obtained by subtraction of the potential heat generated from the feed of the actual heat generated. The level of unconverted reactants over time can be compared for each recipe with a standard profile, and deviation settings for alarming and interlocking implemented. The safeguarding can also be provided by running a real-time model in parallel with the reaction, and comparing the measured and theoretical heat release for deviations. The models used for alarming can be of a simple form, and in general are of the Arrhenius type, with the main contributing reactants and catalyst concentrations applied to the equations. The objective is to measure the conversion to identify potential runaways, and not for product distribution.

8.3.3.1 **Alerting/alarming**

The terms alerting and alarming are defined as follows:

- *Alerting* is intended to warn operators of the start of new transient actions, and any forthcoming deviation of the process.
- *Alarming* is intended to warn operators to take action, because the process is moving to an undesirable situation.

Alerting and alarming is very important in a process plant, and especially so in a simple and robust designed plant. Such a plant is operated with fewer people, but still requires a high level of attention. Potential problems may arise when a situation escalates and alarm "showers" take place, as this leads to confusion of operation at a point in time that rational behavior is urgently needed.

An even more important facet is to keep the operator's attention on the operating process. Therefore, operation must be kept involved in all main operational actions, by demanding various manual actions or confirmations. The target is to "keep operation people alert", and consequently a good alarming strategy is required (Tsia et al., 2000) which includes the following:

- Differentiate between alert and alarming levels
- Prevent alarm “showers” by:
  - assigning alert/alarms to each operational state and transient operation;
  - using an early warning for preventive actions;
  - analyzing control programs for potential situations of alarm showers, specifically during trips and ESD; and
  - keeping operators alert by asking them to carry out certain activities.

The alarm levels are shown in Figure 8.14, where the different alerting/alarming levels – request, alert, pre-alarm, and alarm – are shown in relation to the control levels.

Requests are primarily implemented to involve operation; typical requests are a permission to start with a certain transient operation (not described here):

- Recipe change for a batch process
- Switch from one operational set-up to another; for example, lining up adsorption beds from regeneration to adsorption
- Start of a transient operation, including a shut-down sequence
- Start of a critical unit, such as a reactor or a furnace

Other requests can be formulated to enforce operation to certain actions, such as checking the performance of a certain unit, or analyzing the frequency signal of a measurement to diagnose for pump or valve cavitation.

Alerting is applied to notify operation of deviations between a measurement and a set-point, while the process is still in its normal operational range. This is often applied during a run state to warn the operators of a deviation. The alerting alarms are typically step-dependent. These are also applied during a transient deviation, but with a wider range to prevent over-alerting for what is normal in that transition.

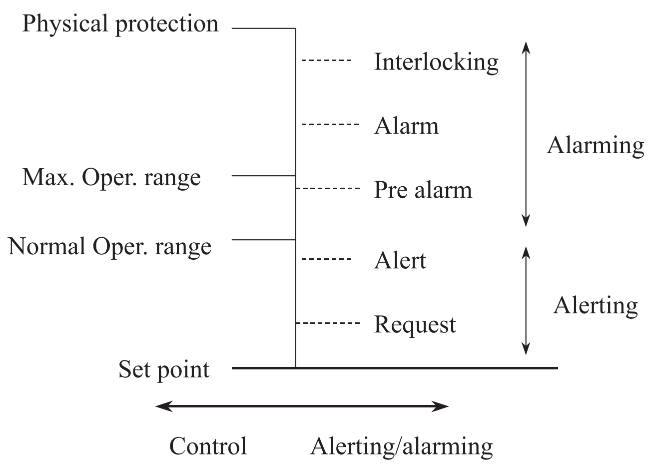

Fig. 8.14. Alerting/Alarming levels in relation to control levels.

(*Pre*)*Alarming* is applied when the process approaches an undesirable condition which requests operator action. An example is the danger of an overflowing storage tank; this requires operator intervention before interlocking becomes activated. In such a situation the control measurement could provide a pre-alarm, while an independent measurement with a higher alarm setting would generate an alarm.

8.3.3.2 **Interlocking**

Instrumental selection, as was discussed for safeguarding, was based on the analysis of equipment which in general forms part of a unit operation. Active protection of the equipment results mostly in interlocking/tripping of any complete unit operation that has been activated after an alarm. In consequence, the process might be severely upset or require part or even complete shut-down or an emergency stop. This problem should be faced during development of the operational strategy, as discussed previously. Different levels of interlocking or trips include:

– Equipment trip
– Unit trip
– Plant shut-down
– Emergency shut-down (ESD)

A *trip* may cascade down through a process plant; hence, these "cascades" need to be foreseen and sufficient instrumentation made available to guide the impact of a trip.

In order to enable smooth start-up of the facility after a trip, this (preferably) would be absorbed in a normal shut-down. An *emergency stop* of the process is generally the result of a major mechanical failure with a serious release or with utility losses that might be manually or automatically activated. The process is automatically blocked, and all actuators are in a foreseen passive failsafe position.

After a trip, emergency block valve (EBV) positions must be confirmed in their failsafe positions by installation of DIs. This is because EBVs are not in frequent use, and their correct functioning in an emergency situation is critical.

8.3.4
Observation

For a simple and robust process, surveyability of the process is very important. Operators are transformed to operation supervisors and need to have limited, albeit good, information on which to judge whether the process is operating as required. It is not only data that needs to be communicated – access to these data is also very important. Given that important information is received, operation also needs to be able to analyze the information and to take appropriate action. Therefore, observability is an important point to address, and comprises the following items:

- Process measurements for overviewing the process.
- Layered redundant control system.
- Layered overview of the process on the panel or screens within ergonomic requirements.

- Consistency and accessibility of the software for interpretation of its operational state and its transient operation.
- Requests for operation attention to see keep them alert..
- Overview of the actual process plant using television monitors.

Instruments for observation are important, as these are planned to inform operators at an early stage if there are deviations from the normal operation. This information can be split into measurements of the process and unit operations, and the following information should be readily available:

- The operational state – that is, the state or its transient operational step at which the process or unit is functioning.
- The line-up – this is especially important for batch operations as well as continuous processes if different line-ups are involved.
- The condition of a units – this should not be confused with the fact as to whether the unit at the desired quality specification (such information is available from the controlled variables).
- The performance of the process

The *operational state* of the different units needs to be clear at a single glance for the operator. For clarification, the following questions may cross his/her mind:

– During a batch reaction, what recipe are we producing, what is the current feeding steps and which are planned for the reaction?
– During start-up, which units are in reversible operation, and which transition steps are active?

For *line-up*, these have questions might be:

– Which loading stations, storage tank or feed tanks are lined up?
– Which adsorber is lined up for regeneration?

The *operational condition* is, next to its quality performance as measured by the controlled variables, directly traceable from some measurements in the units, these being quite sensitive to small operational variations:

– Whether the condition from a distillation column can be read from a pressure-compensated temperature measurement in the column. This might warn operation of any build-up of intermediate component(s) or of any change(s) in feed composition.
– What is the location of temperature front in the absorber? A decrease in inlet concentration might create a breakthrough due to the characteristics of the absorption isotherm.
– How does the radial temperature profile appear for the packed bed reactor?
– How steady is the process? For steady-state, optimization measurements are installed to verify the steady-state of the process before the optimization sequence commences (see **Chapter 9**).

The *performance* of the process covers questions for which, in the past, the answer was hidden from operators. Supervisors performed calculations by hand at their desk, and this was not the concern of operators. Nowadays, the role of the operator is shifted to operational supervisor. Consequently, the information that he/she requires must provide the answers to questions such as:

– What is the compressor efficiency?
– What is the vibration level of the compressor?
– How does the steam balance appear? Do we need to modify the situation by changing turbine operations?
– What is the overall performance of the process expressed in performance terms? (See **Chapter 9** for process performance (profit) metering.)

The required information, in turn, requires some additional instruments. For process observation, these are AIs and DIs, and the instrumentation to provide this information is in addition to the instruments needed for control, operation, and safeguarding.

Note that the installation of (as standard) two switches (DIs) to detect valve position for observation is recommended not only in specific cases (e.g., safety), but also in case of unreliable valve operation (e.g., fouling and high temperature gradient situations). High-voltage switches are, due to their specific nature, provided with DIs in the off position.

8.3.4.1 **Instrumentation Systems**

These form the basis for observability of the process. The design of these systems is undertaken by excellent companies which spend a great deal of development time and money in order to maintain standards. The requirements for this include:

- Current trends to operate several plants (or a total site) from one control room accelerates the need for commonality in instrument systems and software design.
- Avoid the installation of different workstations for different activities, or this can – and will – lead to errors by operation.
- Instrument system should have highly powered floating point processors with programmable operation stations for process observation.
- Instrument systems must perform sequence control, as well as all their controller functions.
- Ergonomics requirements must be respected in the control room to improve observability.
- The reliability of these systems is high, and the technical abilities to provide good on-screen process overviews are excellent. However, attention must be paid to redundancy on power supply. You will never forget being in a control room where all the screens went black due to a power outage!
- The SIS and BPCS (basic process control system) are largely physically separated. Currently, some overlap is considered to be an advantage due to an increased level of knowledge in BPCS. An example is the alarming and interlocking of reactive exothermic systems based on process simulations.

8.3.4.2 Software

In having to execute all the program tasks for which it is designed, software is an important facet of a totally automated plant. Thus, on listing the required qualifications, the following question(s) should be asked as to whether the current software meets these requirements:

- Software development is based on a well-documented operational and control strategy and operational procedures.
- Soft ware should be easy to program, with an accepted high-level language.
- Standard tool kits for common parts need to reduce programming time, and make it easier to adapt the program.
- Common software configuration should be used on the different processes operated from the same control room.
- Software code should be understandable but protected from the operator, and different protection levels must be foreseen.
- A database should be present to enable working with recipe tables for different operational options.
- Different control levels need to be visible in a clear overview, so that the operator knows which level is active and what is its objected functionality.
- Control software needs to handle from simple up to more complex predictive model-based controllers within the same working environment.
- Software testing should be performed for logic by means of a quasi simulation (Fujino et al). Detailed realistic dynamic simulations are required for testing critical dynamics such as model-based alarming or complex model-based controllers. Control parameters can be determined on a preliminary basis using closed-loop dynamic simulations.
- During operation, an operator needs to have immediate access to the software statements that determine its current (non)action. A hold-up in a progressing step should be explained to the operator.
- All operator actions need to be registered.

In conclusion, the selection of instrumentation is based on analyzing control, operation, safeguarding, and observation. The tendency is to over-instrument a process plant, which in turn increases the likelihood of failures resulting in nuisance trips. Nonetheless, there remains a drive for more instrumentation, and everybody adds instruments during the development of P&ID. It is important to re-emphasize the point that, based on the above findings, redundant instruments should **not** be installed unless determined by safety or environmental requirements. Neither should the performance of **all** units be measured routinely – only those that are critical to the operation in terms of economics and reliability. As a yardstick for measuring the degree of instrumentation, the ratios of input to output can be used.

The ratio between analog inputs and outputs (AI/AO) and digital inputs and outputs (DI/DO) can be used as a basis for comparison in instrument design. For continuous processes, an AI/AO ratio of 1 is the ultimate minimum, but in practice a value of less than 3 is achievable. In cases where a reaction occurs in a packed bed, and where local temperatures may lead to hot spots, the ratio may become higher.

The DI/DO ratio (hardware) is dominated by the amount of limit switches on valves and motor drivers, and a ratio of 1 should be easily achievable (this is based on the assumption that are not two DIs per DO).

8.3.5
Summary: Automation of Operation

The approach to a simple and robust plant is one of hands-off operation. The reasoning behind this is that human beings also have, next to their superior function in nature, certain disadvantages. In the operation of process plants they require certain characteristics that are not always available. The consistent performance of tasks is one weak point; they also do not have a good memory, and if something is complicated they are not always going to figure it out. This makes human beings less capable for the operation of a simple and robust process plants. Such a plant leaves less freedom for interpretation during operation, despite the drive for consistency and high-quality production. Thus, the ultimate concept for these plants is one of *total automation*, and in this respect the role of the process operator is changing to that of process supervisor. Automation is based on an operational strategy which is reflected in instrumentation selection and implementation operational procedures.

- Instrument selection is based on the following key elements: selection of CVs and MVs for control, automation of operational actions and start-up and shut-down trajectories, safeguarding, and observation.
- The operational strategy requires:
- – A set of operational objectives which provide safety and environmentally sound production, and total quality control with first-pass prime production.
- – A layered structure of operational states which have to be passed in a defined safe order.
- – Defined transient operations to bring the process safely from one operational state to the next.
- – A set of detailed operational procedures.
- For the operational states, the difference is between reversible and irreversible unit operations.
- – Reversible unit operations are units which can be operated in a stand-alone mode.
- – Irreversible units are started by supplying an appropriate feed and discharging the effluents to downstream units.
- Start-up of irreversible units for FPPP requires: conditioning of the unit, mostly with recycle streams close to its operational conditions, and implementation of trajectory control on feeds and operational temperatures. The design of the optimal trajectories for start-up might be based on experience, but at best is based on dynamic simulations.
- An overall start-up procedure is developed for continuous process plants; this methodology has been verified for three processes.

- Safeguarding is based on the following philosophies:
  - Prevent a potential problem by elimination or minimization of the hazard.
  - Prevent loss of containment by equipment failure.
  - Prevent the release of hazardous chemicals.
- The safeguarding approach is based on:
  - Building different protection layers.
  - Designing inherently safer processes based on the keywords: *Minimize, Substitute, Moderate*, and *Simplify*.
- The direct protection of a process is applied in the following order:
  - Process design by minimizing, substitution. Moderation.
  - Basic control.
  - Alarming.
  - Interlocking (SIS).
  - Physical protection (relief devices).
- Safety instrument system design needs to follow IEC 61508.
- Automated exothermic and gas-releasing reaction systems specifically require safeguarding during transient operations. The design of these safeguarding systems requires dynamic understanding and monitoring of the reactions to enable timely response.
- A layered alerting/alarming strategy was discussed which should have as important elements, keeping the operator's attention by requesting operational confirmation or actions, differentiation between pre-alarming and alarming, and prevention of alarm showers.
- Observation of the process requires:
  - Selected measurements for process monitoring in addition to control, operating and safeguarding instruments.
  - Layered instrumentation system divided into: basic control with interlocking, model-based control and optimization, with the basic control layer functioning independently of the higher control layers.
  - Observable layered flowsheet continuously updated with latest measurement readings, and its history.
  - Layered verified software with an understandable notation for operation and specifying the conditions and process limitations during operation.

Overall instrumentation levels can be judged on the ratio of inputs and outputs. An AI/AO ratio of 3, and a DI/DO ratio of 1 must be achievable.

8.4 Control Design

The achievement of a simple and robust process plants places stringent demands on process control, as one of the characteristics is hands-off operation with no operator in the control loop. The demands on controllability is increased where controllability is defined as:

"The ease with which a process can be controlled to achieve a desired performance within specified limits determined by capacity, product quality, and environmental and safety constraints" (Bogle, 1989).

The developments to support hands-off control has undergone major progress during recent years, and this is reflected by the large number books on control and control design (e.g. Liptak, 1995; Marlin and Hrymak, 1997; Luyben et al., 1998; Skogestad and Postlethwaite, 1996). It is also reflected in the attention given by Seider et al. (1999) in his book *Process Design Principles*, which include chapters on plant wide controllability assessment.

The design of control hierarchy requires a layered approach – also called a decentralized approach – as was illustrated in Figures 8.1 and 8.2: Wolff et al 1992. This concept, which is generally accepted as the basis for a robust operated process, demands a very robust basic control layer which can be easily handled by operation, in case the model-based and optimization layer are not functioning properly and are switched off. The operation needs to proceed hands-off, at some appropriate distance from its constraints and its ultimate optimum operational point. The model-based control layer is designed for multi-variable controllers to de-couple interaction and to approach constraints and support optimization of operation. The inputs and outputs always pass the basic control layer, where the output are set points for basic control loops to ensure independent operation of the basic control layer.

Major progress has been made in the design of a robust basic control layer, which found a basis in the following developments:

- Availability of robust, equation-based dynamic simulators, with extended library models for unit operations.
- Development of a method for plant wide control (Luyben et al., 1998).
- The design methodology for selecting the dominant control and manipulated variables based on a thermodynamic approach (Tyréus 1999).
- The design methodology for self-optimizing control which minimizes interaction by selecting appropriate controlled variables based on economics terms (Skogestad et al., 1999).
- Control strategy selection based on static and dynamic interaction parameters used for selection.
- Implementation of selected control strategies in a simulation for testing robustness and control algorithms on disturbance rejection.
- Development of de-coupling algorithms at basic control layer preferable by algebraic equations (Verwijs, 2001).

The technology developed from heuristic design methods to more fundamental, model-based design methods. These developments still based on linear controllers are the cornerstones for the design of a robust basic control layer.

During the past few decades, most of the control developments have concentrated on the development of multi-variable, model-based controllers. These developments were focused on the de-coupling of interactions and model predictive constraints control. Several types of model-based controllers were developed, including neural net controllers, dynamic matrix controllers (DMC; later extended to Quadratic

DMC), and fuzzy logic control (for an overview, see Qin and Badgewell, 1997). All these techniques require the development of models through process identification (also called input and output models). Compared to fundamental, model-based controllers, these are handicapped by their accuracy. They can be totally out of order in case new conditions occur, such as other feed streams for which the models were not trained, or in case insufficient data are available to achieve a model of sufficient accuracy. However, they have as an ultimate advantage the tenet that detailed process knowledge is not required. The development of hybrid models was expected by Qin et al. (1997). Hybrid models integrate steady-state, non-linear, first-principles models with dynamic empirical models. The ultimate solution is based on the development of dynamic models which undoubtedly will evolve. The disadvantage of dynamic simulation as a time effort will disappear. Dynamic simulations will become easier to program, while object-oriented programming and robust library models will become available. Long execution times of the simulations will completely disappear as computer power is increased progressively. Another argument which plays a role is that modeling technology leads to improved process knowledge. The process knowledge required is very helpful to design more integrated processes which have to meet increased demands on safety and environmental requirements, which as such must result in robust control.

The objective of this section is to describe a methodology for robust control design of the basic control layer, based on fundamental models – static as well as dynamic. A fundamental approach is preferred, as in the long term this will be the only structural way to achieve consistent robust control designs. Nevertheless, historical results have been achieved using an heuristic approach.

8.4.1 Control Strategy Design at Basic Control Level

The basic control layer is dominated by feed-back loops, eventually provided with feed-forward actions to cope with disturbances. The basic control layer will include some cascaded control loops and simple models, such as for de-coupling of interactions, and heat and mass balance control options. The demand on control, next to hands-off control, is higher than in the past due to:

- more stringent requirements on product quality;
- elimination of intermediate storage as lot tanks, check tanks/hoppers and minimization of storage, (implementation of JIP, TQC, and FPPP);
- high level of process integration;
- switchability of process conditions for campaign operations (switchability is defined as the ease with which the process can be moved from one stationary point to another);
- predictive alarming and interlocking actions need to be incorporated to assure safe operations (see Section 8.3.3);

- self-optimizing control of units applied for; stand-alone units and at intermediate time spans between implementation of closed loop steady state operation optimization set points; and
- bases for model predictive control and closed loop process optimization.

To achieve robustness it is vital that any basic model applied for control is preferably solved by an analytical technique. Iterations and optimization are to be avoided, as these might fail in finding a solution unless sufficient provisions are made.

Control design requires a controllability analysis to select the most robust control solution. The result of the analysis may include the need for process modifications to enable control, reflecting interaction between process design and control design. The procedure is based on the latest development in control design and includes the work from Luyben et al. (on plant wide control), Tyréus (on selection of dominant variables on partial (basic) control with a thermodynamic approach), self-optimizing control of Skogestad (1999), and the controllability analysis procedure of Seider et al. (1999).

A procedure for controllability analysis of a process plant has the following sequential steps as presented by Seider et al. (1999):

1. Define control objectives.
2. Evaluate the open loop stability of the process based on static models.
3. Divide the process into separate process sections; be aware that a process section must include a recycle stream from another section, as applied for reactors with unconverted reactants.
4. Determine the degrees of freedom (DOFs).
5. Determine preliminarily the controlled, manipulated, measured and disturbance variables.
6. Determine feasible pairing options in respect of plant wide control and unit control.
7. Evaluate static interaction of the selected pairing options.
8. Evaluate dynamic interaction of the reduced set of selected pairings. In case of evaluation of the controllability during process synthesis this information is input for the final flowsheet selection.
9. Establish the final pairing and design the controllers.
10. Tune and test the performance of the controller in a dynamic simulation.

An overview of the development activities for control design at the basic control layer is presented in overall format in Figure 8.15.

8.4.2
Definition of Control Objectives

Definition of control objectives for a total process operation is; to maximize the profits by converting raw materials into products which have to meet quality specifications while respecting safety and environmental requirements and operational constraints.

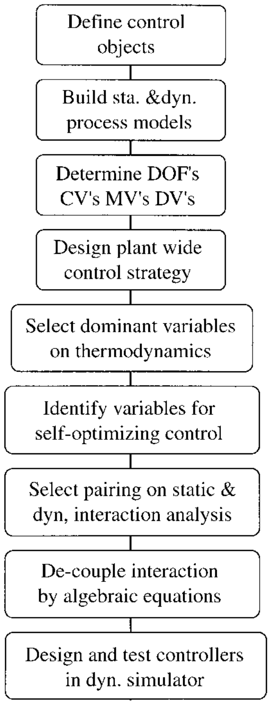

Fig. 8.15. Control design activities for a robust basic control layer based on first principle models.

The control objective for the basic control layer is restricted in the decentralized control concept. The opportunities for process optimization and constraint control are reserved for the higher control layers. Therefore, the control objective for the basic control layer is defined as: Robust control of a process plant under defined process condition of operation, by setting master set points for capacity, feed, product mix and specifications, for a selected level of disturbances while respecting safety and environmental requirements and operational constraints. Respecting safety and environmental requirements must be interpreted as: initiate action in terms of alerting, (pre)alarming and interlocking actions to comply with these requirements, in case normal control actions are insufficient. Operational constraints are process conditions where the process would not be able to function optimal by exceeding. These conditions include capacity limits and temperature limits. The definition does not exclude self-optimizing unit control (to be described later) as practiced at the basic control level.

8.4.3
Evaluate Open Loop Stability

A controllability study is started with the determination of the open loop stability– through perturbations of static process simulations around the operating point(s). Normally, we like to avoid open loop unstable designs. Process modification, mostly around exothermal reactions, might result in a unstable open loop design this can be made stable by adapting the heat removal systems. Sometimes these situations are difficult to prevent, in which case the hazard is often minimized by changing the operational conditions to limit the reactants inventory and its concentrations. A typical example is the redesign of a batch reactor into a continuous-fed batch reactor design.

8.4.4
Divide the Process into Separate Sections

The intention is to reduce the control design problem. The subdivision should be done in such a way that relevant recycle streams are included, such as a recycle from the finishing back to the reactor. It would not be relevant if an incremental recycle simply replaced a small part of a fresh feed stream. In case the recycle would contain some impurities which might impact on the reaction or the finishing train and would build-up, this needs to be considered. A similar situation might occur with heat integration. When this is provided with a back-up (as in Figure 4.29 in **Chapter 4)**, it is not considered relevant for the separation sections (although it will still appear as disturbance). The disturbance must be absorbed, as was shown in the example of the heat exchanger with heat balance control.

8.4.5
Determine the Degrees of Freedom

The degree of freedom analysis is the first step before the selection of the variables. The following equation has been derived:

$$N_{DOF} = N_{Variables} - N_{Equations}$$

where N_{DOF} is the number of degrees of freedom, $N_{Variables}$ is the number of process variables, and $N_{Equations}$ is the number of independent equations that describe the process.

The number of manipulated variables of is less than the number of DOFs, as some variables are externally defined:

$$N_{DOF} = N_{manipulated} + N_{External\ Defined}$$

where $N_{manipulated}$ is the number of manipulated variables, and $N_{External\ Defined}$ is the number of external defined variables.

Now, the number of independent manipulated variables is:

$$N_{manipulated} = N_{Variables} - N_{External\ Defined} - N_{Equations}$$

The number of independent manipulated variables is preferably equal to the number of controlled variables that are controlled. When a manipulated variable is paired with a controlled variable (control loop), the DOF is transferred to the set point

The number of MVs is not always equal to the number of CVs This can be solved from two sides. Sometimes, an additional MV can be created; for example, when the duty of a heat exchanger cannot be controlled, a bypass might be provided. Another example is when a feed composition has a relevant impact on an controlled variable, a separate feed system might be installed. Another option to be explored is to evaluate the CVs carefully, as on occasion we simply do not have any capability to control it – in which case it needs to be removed or solved in a multivariable, model-based environment.

8.4.6
Determine the Controlled, Manipulated, Measured and Disturbance Variables

Manipulated and controlled variables are respectively input and output variables which can be selected by qualitative criteria as formulated by Newell and Lee (1988).

Controlled variable (CVs) selection might preferably follow the guidelines:

- Select variables which are not self-regulating; variables which result in a new steady-state situation without a feed-back control should not be selected. An example of a self-regulating system is an hydraulic overflow system. As is often applied in decanter systems, this is termed a simple self-regulating system.
- Select variables which exceed the constraint of the process. Safety constraints, as well the tendency to operate close to its constraints under optimized conditions, requires that controlled variables are selected which exceed the constrained values.
- Choose variables which directly measure the condition and quality of the process streams, or that have a strong relation to it. As composition measurements are expensive and often have long response times, the preference is to select variables that are easy to measure with short response times, but which have a direct relation to the property of interest.
- Selection of output variables which have a significant interaction with other controlled variables are preferred. Closed loop performance is improved by stabilizing control variables which interact significantly.
- Select output variables which have favorable static and dynamic responses compared to other controlled variables.
- Variables selected for control should not correlate too closely.

The selection of manipulated variables (MVs) must follow certain guidelines:

- MVs must affect the CV strongly, which means that it requires a large steady-state gain. This results in rapid responses and less variations in flow of the manipulated stream, and less potential impact on other units.
- Operational range of the manipulated variable is a characteristic which need to be respected. A bypass valve around a heat exchanger might give a limited controllability of the exchanger duty.

- MVs are preferred which have a direct effect on the CV. A direct effect on a CV results in fast responses, which are preferred. The removal of inert from a condenser works rapidly and more effectively than an increase in the cooling flow.
- Avoidance of recycling disturbances. Disturbances are at best prevented, but when they are introduced they should leave the process through its exit streams. When disturbances are recycled or feed streams are manipulated, they have a larger impact (see disturbance variables).

Measured variables are to be selected by the following guidelines:

- Measured variables must reflect the CVs. Preferably, do not measure the volumetric flow when you want to control the mass flow. Temperature measurements representing dual composition in a distillation column require pressure correction.
- Measurement should be reliable, robust, and accurate, and have a sufficient operational range.
- Location of the measurement should be sensitive to a disturbance. Pressure measurements should be at the compressor, and not at downstream or upstream units. Temperature measurements should be installed where variations are observed at first, such as in a steep temperature transient in a distillation column, or at the front end of a plug-flow reactor.
- Measurements should minimize time delays and time constants. This is determined by the type of instrument, the location, and any sampling system.

Disturbance variables (DVs) are selected for testing the robustness of the designed control configuration, but they must be minimized by appropriate action. Disturbances can be split in internal disturbances and external disturbances:

External disturbances are:

- Weather conditions, as day and night temperature cycle, humidity variations for cooling water systems, rain showers. Atmospheric conditions changes over a longer time period (daily or weekly or even seasonally are not experienced as a disturbance) are not experienced as a disturbance for control of the process system which mostly have hourly or shorter response times.
- Feed conditions and compositions.
- Utility conditions.

Internal disturbances are:

- Economical disturbances which determine capacity, product distribution, internal quality set points, equipment scheduling. These are grouped under internal disturbances as the implementation of modified conditions is under operational control.

- Operational disturbances are caused by operational activities; for example, when units or components are taken in or out of operation for cleaning, regeneration, or repair. Even if these activities are automated, they are still to be recognized as a disturbance.
- Control disturbances which cause propagation or even amplification of a disturbance through the process system, particular so for recycling of disturbances. These are negatively influenced by; inappropriate control design, and wrong tuning of control loops.

The impact of both types of disturbances can be handled in different ways they can be categorized as:

- Prevention or limitation of a disturbance is a preferred action, examples are:
- – Design internal utility grids less sensitive to external (site) variations by operating the internal system with a pressure controller slightly above or below the external grid level, depending on an import or export situation.
- – Inventory with mixing devices will minimize composition or temperature variations.
- – Smoothly ramping of set point changes particular for flow, pressure and temperature and economically determined set points
- – Gradually and smoothly taking units in or out of operation
- – Design for back-up supplies like is applicable for heat-integrated systems (see Figure 4.29 in **Chapter 4**).
- – Correct for any concentration variation of a feed stream. For example hydrogenation reactors often need to control the mass flow of hydrogen, this means correction for any impurities is required.
- Rejection of disturbance to outside the process is easily applied for utility systems and inventory feed systems. Examples are:
- – Any deviation in utility consumption such as steam is exported to external supplies. Site utility systems are normally designed with short response times to enable fast compensation of demand variations.
- – Reactors experience changes in conversion which have an impact on recycle flows, and as such varies the demand on feed of reactants. These variations can be absorbed at the supplier, or in the inventory.
- Absorption of disturbances depends on process design and control design. Examples are:
- – Inventory in reactors, column bottoms, reflux drums and surge drums to smooth variations in flow and/or composition.
- – De-coupling of interactions to direct a disturbance outside the process and avoid recycling or transmitting to other process sections.

These three methods for disturbance handling should be recognized and exploited in sequential order of the above discussion and in full understanding between process and control designer. Design modification might be essential to limit the effect of disturbances.

8.4.7 Determination of Feasible Pairing Options in Respect of Plant Wide Control and Unit Control

Different types of control functions can be recognized, all of which have their place in the control design of the process plant. These can be divided into:

- Inventory control, mainly level and pressure control.
- Capacity control, which includes product distribution.
- Quality control for products.
- Constraint control, mostly executed at MBC level but also at basic control level (see Figure 9.14 in **Chapter 9**) for floating capacity control.
- Economic control, like set points for: conversion control of reactors and quality set points for recycle streams. These are normally calculated at the optimization level and implemented at the basic control level.

The design of the control configuration reaches it critical point now, when CVs, MVs, DVs and measurement variables have been preliminarily identified. The final identification will take place during the design of the control configurations, as detailed analysis might lead to alternative CVs or MVs to achieve the same control objective. There are two separate points which must be addressed and are differentiated as plant wide control and unit control.

8.4.7.1 Plant wide process control

This is extensively discussed by Luyben et al. (1998). Plant wide control approach is also a step-wise procedure which in essence starts with the external (site) situation. This places constraints on the control design, utility wise, as well as on the feed and product sides. In a similar way, plant control design places constraints on unit control design which must be respected. The design steps as set out by Luyben et al., and which fit into this sequential step for selecting feasible loop pairings, are as follows:

- Establish an energy management system. Crucial in this respect is to avoid propagation of disturbance in the energy systems which are transferred to the different units in the process. This can lead to total plant swings – which are to be avoided. The determination of operational conditions of the plant utility levels and provisions for back-up supply are essential. It was concluded previously that the rejection of disturbances outside the plant is a good solution, as most utility systems are designed to cope with fast load variations. The impact and priority within the site load shedding systems need to be reflected in the control design of the system.
- Set production rate includes also the required product distribution. The production rate for batch plants is determined at the front end of the process, which is designed for feed-forward control with some limited feed-back actions. Recycles are collected and processed for next batches. For continuous processes, the production rate might be set by a flow rate between reaction

and finishing section. So, the front end and the back end of the plant are stabilized when the reactor is conversion controlled. Such a control design minimizes swings in recycle flow and puts any disturbance in recycle up-front to the feed supply system while maintaining the reactor feed constant, see also below under set recycle streams.

There are many production plants where the feed flow is set (e.g. in olefin plants), and this is determined by furnace loads. In those situations recycle flows are not fixed, but some intermediate recycle storage is quite often foreseen to accommodate a more constant recycle In exceptional cases a downstream plant sets the production rate of an up-front process; this has been done for gaseous supplies, but it places a constraint on the supplier plant control design.

- Conversion control of the reaction is essential from control stability perspective not limited to the reactor section, but for the whole plant. It also sets the product distribution while its set point represents the economic trade-off between conversion costs and selectivity. The conversion of a reactor requires selection of the dominant variable for control; the factors which have to be considered include temperature, residence time, reactants and catalyst concentrations, pressure, and mass and heat transfer rates. The selection of the dominant variables can be done by evaluating all relevant variables in a static reactor model. The selection of dominant variables based on a thermodynamic methodology is discussed later in this section. An accurate, reliable and fast responding conversion/composition measurement at the outlet of the reactor is a requirement.
- Control of product quality within safety environmental and operational constraints. Quality control is mostly achieved at unit level; however, these can be divided into separation units and reactor units. An example of product qualities which are determined at reactor level are hydrogenation reactors – either selective hydrogenation such as C2 and C3 hydrogenation to remove acetylenes and di-olefins; or total hydrogenation such as nitrobenzene, which is totally converted to aniline. The design of the control structure for quality is discussed under unit control.
- Set the flows for recycle streams and determine inventory control (pressure and levels) It is (according to Luyben et al., 1998) fundamental to fix recycle flow for a process plant. It was said earlier that disturbances, when neither prevented nor rejected, need to be absorbed. Absorption is done by inventory control, where flow and composition variations are smoothened or to propagate the disturbance directly outside the process in process or utility streams; in the latter case it is often also absorbed in an inventory system outside the process. Recycle loops might be subject to large variations if they are not controlled it is what Luyben et al. called the "snowball effect". The sensitivity of recycle loop flow rates to small disturbances can cause large swings in these recycles, which propagates disturbances through recycle flows which are to be prevented. The solution is to fix recycle flows. This is not conflicting with reactor control, which is still controlled by its dominant variables, but the

feed rate can be set in ratio to the recycle. By fixing the recycle flows the process operates very stable. Most hydrogenation reactors, recycle hydrogen over the reactor system and operate at maximum flow rate of the recycle compressor which is a widely accepted control mode, which a way of setting the recycle flow.

Inventory control includes pressure, as well as level. The stream which has the largest effect on the inventory should be used for its control – this is known as the Richardson rule. A well-known example is that of distillation columns with large reflux ratios where the level is controlled by the reflux instead of the distillate flow. For pressure regulation, the cooling duty of a condenser is often selected for manipulation. In case inertia are available, the removal of the inertia has a large effect on the cooling duty, even when it is only a small stream, and so this is often selected.

- Check component balances: it is important to understand these for control purposes, particularly at impurity level. They might come from different sources to be named: introduced with the feed, formed in the reaction, or introduced with additives which eventually might fall apart. They must be recognized specifically for situations with recycles, as they will build up due to their integrated effect, and must exit the system somewhere. Their build up needs to be quantified, and any effect on reaction or separation understood. The places where these components leave the system must be identified, and eventually CVs and MVs assigned for their removal. Also, in straight-through systems it is worthwhile understanding their effect. In such a situation they either must leave the system with product streams (in which case there is an effect on the separation and purity), or a separate outlet (purge stream) must be created, like a vent or side stream. Even when the impurities leave with the products, build up may occur in the separations and affect any quality measurement, like a temperature in a separation column. The concentration levels of impurities might be subject to large swings, and this can handicap operation and control if the mechanism is insufficiently understood. The swings might be caused by varying feed and additive compositions, varying reaction conditions, or by variations caused by control.

Unit control is primarily based on feed-back control, while some cascading and feed-forward action might also be involved. The plant wide control approach must be decided before unit control can be designed. It determines the constraints for the control design next to the operational, safety and environmental constraints. Unit control still offers many opportunities for pairings CVs and MVs. A methodology must be followed to achieve a robust basic control layer which is the objective for a simple and robust process plant. The methodology emphasizes several elements, which are:

- Selection of dominant variables and its pairing for control.
- Selection of self-optimizing control options.
- Determination of static interaction for selected options.
- Determination of dynamic interaction for selected options

During the controllability step 2 of process synthesis this information is required to evaluate different flowsheet options, see **Chapter 4**.
Selection of final control loop pairings and any de-coupling algorithm.

8.4.7.2 Selection of the dominant variables

The selection of the dominant variables can be done in two ways – either by static simulations and determination of the process gains of selected variables, or by a thermodynamic method for identification. Both are analytical techniques which determines the dominant variables for control.

Analysis of different control variables by simulation is a straightforward approach for simple systems where the variables are known from experience. In case of complex reactor systems, it is not always easy to analyze in those cases, and the thermodynamic method for identification might be preferred (Tyréus, 1999). This latter methodology identifies the dominant variables that affect the rate of *energy* exchange within the process. The method is based on earlier work of Schmid (1984) and Fuchs (1996).

The methodology is based on the introduction of the term "substance-like". This is a terminology which describes a physical quantity that behaves like an actual substance, such as the mass of material within a process, the amount (moles) of chemical components, the electrical charge, energy, entropy, and momentum. These substance-like quantities can be characterized by three terms: density; flow; and a balance or continuity equation.

Continuity equations have a production term included in them; however, mass energy and momentum lack a production term. Because these last substance-like quantities are conserved, the production terms are true for entropy and also for components formed during a reaction.

While the balance equations are applicable for substance-like quantities under conceivable conditions, they can only be solved if the production term can be formulated. The production terms are called constitutive equations.
"The constitutive equations describe how substance-like quantities affect the state of a particular dynamic system and how the quantities flow in and out of the system depending on the system state"

When it is accepted that a physical system can be described with balance and constitutive equations, the question is which substance-like quantities should be used to describe the dynamics of a physical system. Schmid and Fuchs provided the answer to this question.

For mechanical systems, momentum was identified as the fundamental substance-like quantity, for electrical systems it was electrical charge. For chemical systems, the amount of component and for thermal systems entropy are used as the independent substance-like quantities:

The amount of energy transported with the flow of a particular substance-like quantity is the product of the quantity's flow rate times its intensity (potential).

The intensity with momentum is velocity, while the intensity for electrical charge is voltage. The intensity for a chemical component is chemical potential, while for entropy the intensity is the absolute temperature. The intensities are a subset of the intensive variables used for equilibrium thermodynamics.

Now reactive and physical separation systems can be described with substance-like carriers. Since energy as such can neither be produced nor consumed, every process might be seen as an exchanger of energy. Tyréus (1999) referred as example to a fuel cell where (entropy flow rate × absolute temperature (intensity)) = power generated by the chemical reaction. Other examples cited were flash and distillative separations. This is summarized as follows: a process system can be described by a generalized balance equations applicable for substance-like quantities to identify variables that determine the rate of energy exchange. For a chemical system, the process can be modeled by the number of component balances and one entropy balance. The balance equations need to complemented with the constitutive equations which depend primarily on the intensive variable (such as temperature, pressure) of the process.

8.4.7.3 Thermodynamics and partial control

Partial control has been defined by Tyréus et al. (1999) as a form of decentralized (basic) control in which the controlled variables are explicitly paired with the manipulated variables such that the main feedback loop are easily identified.
A physical justification needs to be derived to identify the dominant variables from the thermodynamically description of the process. The economic performance of a process is determined by the production rate and the conversion and selectivity performance. During operation optimization, the operational conditions are pushed against their constraints, operational, safety environmental and product specifications to achieve the maximum economic performance. The economic objectives are mostly tied to the flow and production rates of substance-like quantities, and to the intensive variables that help to establish these rates. To use thermodynamic models for guidance in the identification of substance-like quantities, the focus must be on the constitutive equations instead of the balance equations. As a help in the selection of the constitutive equation the *energy principle* was introduced by Fuchs (1996), which is applicable to all process systems. It states that at steady state, the net energy flow in and out of a process should be zero. The energy might, however, flow in and out with different carriers.

> *The internal rate of exchange of energy between the various carriers will thus be taken as the most relevant rate indicator of a process and the process variables affecting the energy exchange will be considered dominant.*

The rate of energy exchange is expressed as the power release expressed in an entropy substance-like quantity for a flash unit (see Figure 4.16) appears as:

$$P_{flash} = I_s\,(T_{out} - T_{in})$$

where P is power in Watts, I_s is entropy current W/°K, and T is absolute temperature °K

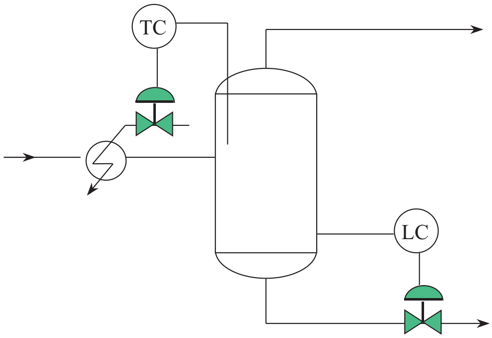

Fig. 8.16. Flash unit with basic control loops.

This expression is the constitutive part of the balance equation. The expression eliminates all the terms of the balance equation like the components terms, and only leaves the essential terms for the operation. It shows for a flash that only three variables affect the rate of energy transfer between the entropy current and the flash temperatures; these are the considered potential dominant variables. The I_s flow term can be manipulated, while the temperatures are the intensive variables. In this example the temperature in the flash is dominant, as the up-front temperature is not available for control in this scheme. The control scheme with the dominant variables is shown in Figure 8.16.

The following *loop pairing rule* was presented by evaluation of the power release term for a unit:

Whenever a flow appears as an important energy carrier pair this flow with the corresponding intensity belonging to the unit.

When this rule is applied to other thermal processes like a distillation column, the energy carrier (heat duty of the reboiler) is paired with a corresponding intensity (selected column temperature). Identical expressions for thermal processes can be generated that are also applicable for single component irreversible reactions such as $A \rightarrow B$ that can easily be expressed as a thermal process (e.g., a fired heater). In a fired heater, the loop pairing is the energy flow and a (intensity) process temperature.

For multi-component reactions the component production terms must be included in the equation. This has been described extensively in the referred article of Tyréus with several general conclusions for irreversible and equilibrium reaction systems.

The methodology has demonstrated its usefulness by its application to a coupled reactor system as a FCC unit. An entire process (Tennessee Eastman process) was successfully studied with this methodology to design the dominant pairings.

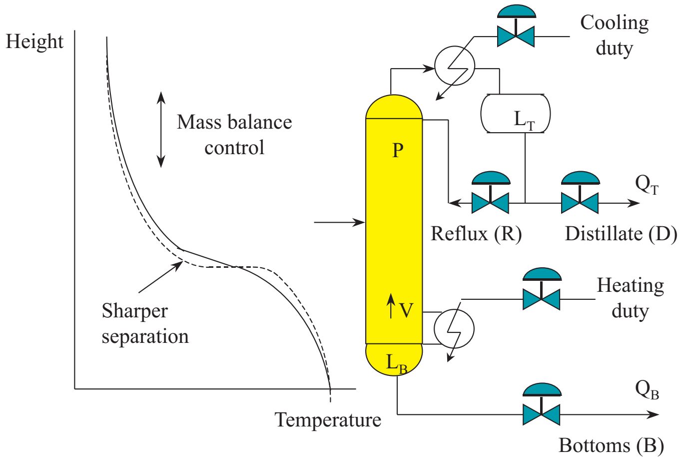

Fig. 8.17. Distillation column with five CV's, MV's and temperature profile.

In the above, the dominant variables and its pairing are selected are selected for unit control. There remain many loops to be closed, such as product quality and inventory loops, which still leaves many options open. These may lead to both static and dynamic interactions, and avoid closure of the loops.

When we return to the distillation example in Figure 8.17, during the dominant variable selection we found that the separation is dominant and influenced by the heat input. A normal distillation has five CVs, which include two qualities Q_T and Q_B, two levels L_T and L_B, and a pressure P. Five MVs are involved: reboiler heat duty (V); cooling duty (C); reflux (R); bottom (B); and distillate (D) valves – hence it is a five-by-five system.

One loop is selected as dominant variable V, while another dominant variable is the mass balance effected by bottom flow B, distillate flow D or indirectly by reflux R. The mass balance control shifts the concentration profile, reflected in a temperature profile, up and down the column, while an increased separation is reflected in a steeper temperature profile.

There are still many pairing options open, and even when pressure is controlled with cooling duty the remaining options are: Q_T by V or D,B, R; Q_B by V or D,B, R; L_T and L_B by D,B,R in this list we did not include reflux ratio as a MV. The question is which is the preferred option for a specific distillation column.

8.4.7.4 Self-optimizing control

A design methodology is discussed based on work from Skogestad et al. (1999) for the selection of the controlled variables to obtain a self-optimizing control structure. Definition:

> *A self-optimizing control structure is designed to achieve acceptable loss with constant set point values for the controlled variables.*

The search for such a structure is of value for unit control, and it is often difficult to close two quality loops (such as for a distillation column) without introducing severe interaction that would require a model-based controller. On the other hand, it is quite common that only one of the objected control values is a hard constraint like a product specification, while the other is economically determined – a so-called soft specification. A third point is that steady-state operation optimizations set points are implemented over a time period of hours or even days for off-line optimizations. In the meantime, disturbances might be introduced which must be absorbed. In these intermediate times the units still need to be operated at close to optimum conditions. The above points were a reason to search for self-optimizing control structures of individual units, reactions and separations, with minimal losses as a consequence of disturbances while limiting the amount of interaction. A typical example of a self-optimizing control structure for a distillation column is a top and bottom quality control. Such a structure however does not comply with the requirement of limited interaction, which is basic for a simple and robust process plant.

Skogestad (1999) presented a step-wise methodology for development of self-optimizing control structures by comparing different options, and illustrated this with examples for reactor and distillation control.

The steps for the distillation example Figure 8.17 (a propylene/propane splitter with 110 theoretical stages) were:

1. The selection of the basic design conditions for reference; the distillate spec x_D is considered as a hard constraint 0.995.
2. Selection of disturbances in the example were feed flow increase of 30%, feed composition z_F from 0.65 up to 0.75 and down to 0.5 parts of lights, decrease in liquid fraction q_F from 1.0 to 0.5 (50% vapor) and a impurity increase of distillate from 0.995 to 0.996. Economic disturbance was reflected in the price of energy, which was increased a factor five from 0.1 to 0.5 \$/kmol boil-up V, the price p for distillate 20 \$/kmol, which was increased to 30 \$/kmol in reference to a feed cost of 10 \$/kmol.
3. Selection of the potential controlled variables.
4. Calculation of the steady-state economic optimal conditions of the distillation for the selected variables and the different disturbances.

The results for the optimized distillation conditions in respect to the selected disturbances are shown in Table 8.4 including the nominal conditions. Some of the conclusions were:

- The values are insensitive to the feed rate (as was to be expected), as the efficiencies are not capacity-dependent, and the feed-forward action implemented for R, D, and V.
- Optimal bottom composition is rather constant, with the exception for the high energy price.
- Optimal values of D/F varied significantly, which seemed to be a bad choice for a CV.

Based on the results, candidate CVs were selected.

Table 8.4. Optimal operating distillation conditions and profit for different disturbances (Skogestad, 1999).

Conditions → ***Disturbances ↓***	***x_D***	***x_B***	***D/F***	***R/F***	***V/F***	***R/D***	***P/F***
Nominal	0.995	0.04	0.639	15.065	15.704	23.57	4.528
F = 1.3	0.995	0.04	0.639	15.065	15.704	23.57	4.528
$z_F = 0.5$	0.995	0.032	0.486	15.202	15.525	31.28	2.978
$z_F = 0.75$	0.995	0.05	0.741	14.543	15.284	19.62	5.620
$q_F = 0.5$	0.995	0.04	0.639	15.133	15.272	23.68	4.571
$x_D = 0.996$	0.996	0.042	0.637	15.594	16.232	24.47	4.443
$p_D = 30$	0.995	0.035	0.641	15.714	16.355	24.51	
$p_V = 0.5$	0.995	0.138	0.597	11.026	11.623	18.47	

D, B, F and V flows in kmol/min; D = distillate; B = bottom stream;
V = vapor; F = feed
prices; $p_{F,\ D,\ B,\ V}$ = \$/kmol; P = profit in \$/min;
z_F = feed concentration of lights; q_F = vapor fraction of feed
Nominal conditions: F = 1.0, $z_F = 0.65$, $q_F = 1.0$, $p_D = 20$, $p_v = 0.1$

Based on the selected disturbances, the losses were calculated for the distillate specification $x_D = 0.995$ and the selected CVs.

The losses are summarized in Table 5. Some of the conclusions were:

– The losses are small when the bottom concentration x_B; is directly controlled, this represents the dual composition control which is self-optimizing, but requires a model-based controller for interaction compensation.
– R is a bad choice, particularly when feed flow variations are involved.
– D/F as well as R/D cannot handle feed composition variations efficiently.
– R/F and V/F appears to be the best choices next to x_B, but they are sensitive to implementation errors.

Selection of best pairing

The three selected CVs for further evaluation are:

1. x_D and x_B
2. x_D and R/F
3. x_D and V/F

The belonging MVs are respectively:

1. V and D,B,R/F or reflux ratio
2. V and R/F
3. R and V/F

Table 8.5. Losses of distillation for different selected control variables at different disturbances (Skogestad, 1999) (Nominal profit $ 4.528/min).

Controlled variable → ***Disturbances ↓***	x_B = ***0.04***	***D/F = 0.639***	***R = 15.065***	***R/F = 15.065***	***V/F = 15.704***	***R/D = 23.57***
Nominal	0.0	0.0	0.0	0.0	0.0	0.0
F = 1.3	0.0	0.0	0.514	0.0	0.0	0.0
$z_F = 0.5$	0.023	infea	0.000	0.000	0.001	1096
$z_F = 0.75$	0.019	2.53	0.006	0.006	0.004	0.129
$q_F = 0.5$	0.000	0.000	0.001	0.001	0.003	0.000
$x_D = 0.996$	0.086	0.089	0.091	0.091	0.091	0.093
20% impl. error of CVs	0.12	infea	0.119	0.119	0.127	0.130

Losses in $/min, D, B, F and V flows in kmol/min.;
z_F = feed concentration of lights; q_F = vapor fraction of feed;
$p_{D,B,V}$ = $/kmol.
Nominal conditions: F = 1.0, $z_F = 0.65$, $q_F = 1.0$, $p_F = 10$ $p_D = 20$, $p_v = 0.1$, $x_D = 0.995$
20% implementation error on CVs; $x_D = 0.996$; $x_B = 0.048$; D/F = 0.766; R = 18.08; R/F = 18.08; V/F = 18.85; R/D = 28.28.

These selected pairings are subject for evaluation after the interaction analysis, see below. After the selection of the final pairing for quality control, the pairing for the inventory control can easily be deduced. For details of the method and the conclusions, see Skogestad et al. (1999).

The methodology for selection of controlled variables based on a self-optimizing control approach, is performed by analysis of steady-state simulations. The methodology which is generically applicable for units follows the following sequential steps:

1. Determine the degrees of freedom available for optimization of the unit.
2. Define the optimization problem as a cost or profit problem and identify the constraints.
3. Identify the most important disturbances. These can be divided into process disturbances as well as parameter disturbances and implementation errors. Variations in price sets are normally not included. These determine the set points for controlled variables which are submitted periodically from off-line or closed-loop process plant optimizations.
4. Optimization of unit for different disturbances. From these optimizations the nominal optimal values are calculated for all variables, including controlled variables of interest.
5. Identify candidate controlled variables.

6. Evaluate losses of the selected controlled variables, which are kept constant, due to disturbances and implementation errors versus the optimal case.
7. Analyze and select the sets of CVs and MVs with acceptable losses as candidates for self-optimizing control. These selected CVs and MVs will be subject for further evaluation after interaction analysis.

8.4.8
Evaluate Static Interaction of the Selected Pairing Options

Steady-state analysis is the first step to evaluate the pre-selected pairings of CVs and MVs on interaction of loops. This is performed by perturbations of the input of static simulations. The functions to be determined are the process gains and the relative gain analysis (RGA). The process or open loop static gain is the change of Δy_i in output y_i relative to a change in Δu_i in input u_j where all other inputs remain constant

$$\left(\frac{\Delta y_i}{\Delta u_j}\right)_{u_{m\neq j=0}}$$

The other outputs may or may not change.

Another open loop gain is defined as the change Δy_i in output y_i relative to a change in Δu_j in input u_j where all other outputs remain constant Also, in this case the other input may or may not change now

$$\left(\frac{\Delta y_i}{\Delta u_j}\right)_{y_{1\neq i=0}}$$

The ratio between these open loop gains defines the relative gain λ_{ij} between y_i and input u_j

$$\lambda_{ij} = \left(\frac{\Delta y_i}{\Delta u_j}\right)_{u_{m\neq j=0}} \Big/ \left(\frac{\Delta y_i}{\Delta u_j}\right)_{y_{1\neq i=0}}$$

In words it is phrased as:

$$\frac{\text{Process gain as seen by a given controller with all other loops open}}{\text{Process gain as seen by a given controller with all other loops closed}}$$

When $\lambda_{ij} = 0$ then y_i does not respond to u_j and should not be used to control y_i.

If $\lambda_{ij} = 1$ then y_i does not respond to any other $u_{m\neq j}$ and the loop is not affected by other loops this is the preferred case If $0 < \lambda_{ij} < 1$ or $\lambda_{ij} > 1$ then interaction is present. The more that λ_{ij} deviates from 1, the larger the interaction.

Now, the level of interaction can be determined by putting the relative gains in an array, called RGA which is a square matrix. For multiple inputs and outputs

$$\begin{array}{cc} u_1\, u_2 \ldots u_n & \\ \Lambda = \begin{bmatrix} \lambda_{11}\lambda_{21}\ldots\gamma_{1n} \\ \lambda_{21}\lambda_{22}\ldots\lambda_{2n} \\ \vdots \\ \lambda_{nl}\ldots\ldots\ldots\lambda_{nl} \end{bmatrix} & \begin{array}{c} y_1 \\ y_2 \\ \\ y_n \end{array} \end{array}$$

From the RGA matrix the control loops can be selected by pairing the controlled outputs with the manipulated inputs in such a way that the relative gains are positive and as close as possible to unity. The RGA must be complemented with dynamic interactive control analysis.

8.4.9. Evaluate Dynamic Interaction of the Reduced Set of Selected Pairings

Dynamic models are the bases for the development and testing of robust controllers. These controllers might also include models based on algebraic equations to decoupled loops or support feed-forward and feed-back actions. Dynamic simulations have some specific requirements. Dynamic model building is nevertheless the availability of unit library models, still time consuming. In general reduced versions are made of the static simulations. As control studies do not require the same level of detail, while the studies concentrate around a steady-state operational point where discrete event are avoided. An exception is that of the models for batch processes, which have to simulate discrete events.

Model reduction The number of components is often reduced in as much as they do not play a major role regarding dynamics of the system. They are kept in the simulation when they:

- have a significant effect (negative as well as positive) on the reaction;
- are key components for separations; and
- are accumulated in the system and need to be specifically removed.

Reactor models are quite commonly reduced to conversion models (Verwijs, 1992, 2001, although when product properties must be controlled (as in polymer processes), components cannot be excluded.

Distillation models can be reduced by lumping trays of towers. A large effect on the size of the model (much less equations) for a distillation tower are achievable when the number of trays are reduced by lumping and the number of components reduced.

Heat exchangers are normally not dynamically simulated, but in the case of heat integration this might be a requirement, particularly so when there is no back situation (as provided in Figure 4.29 in **Chapter 4)**. Due to their fast dynamics in relation to other process dynamics, pressure control is in general not dynamically simulated; neither are level controllers.

Some designers work on black box models derived by mathematical model reduction techniques from fundamental models these are less transparent and should, to authors opinion, not be used for control strategy design. With these models the process insight is lost – you could call this designing in the dark. Although these models find useful application in model-based controllers designed to save run time in a real-time environment.

The objective of the dynamic simulation is to design both control strategies and controllers, and this requires a reasonable accuracy of the dynamics of the models.

The validation of reaction and separations for static models have been addressed primarily by process designers. Dynamic models require a realistic representation of the dynamics for the control designer. Key factors for evaluation are the response time, dead times, and related time constants next to concurrency on process conditions However be aware that any large response time of measurements is included in the simulation. Measurements on similar equipment can provide a good indication of these time parameters. Although an error of 15% on response times still forms a relatively good basis for control design, controllers can still be adjusted within the process.

There are several different types of dynamic interaction analysis, and these are outlined only briefly at this point (Skogestad, and Postlethwaite 1996).

- The RGA can be expressed as the sum norm (sum of the absolute values of all elements) of the RGA matrix minus the identity matrix:

  $\|RGA - I\|_{sum}$

The identity matrix is the ideal RGA matrix if the inputs and outputs are arranged in such a way that the preferred pairings are at the diagonal. The RGA number therefore gives a quantitative measure of the non-ideality of the RGA matrix, and can be used to check whether the steady-state pairing holds over the frequency range where control is needed.

- Dynamic RGA, (McAvoy, 1983).
- Singular value decomposition.
- Condition number – this is the ratio between the gains in the strong and weak directions

  $\mathrm{CN} = \overline{\sigma} \big/ \underline{\sigma}$

A system is said to be "well-conditioned" if all output directions can be realized with roughly the same effort as for the inputs. A high condition number indicates that the system is ill-conditioned. Some combinations of the input have a strong effect on the outputs, while other combinations have a weak effect. A condition number of 1 is the preferred situation.

- Morari resilience index. The minimum singular value of the plant is a useful measure for evaluation the feasibility for achieving acceptable control, (Morari and Zafiriou, 1989)
- Performance relative gain array, PRGA.
- Static disturbance gain matrix. The static disturbance gain matrix G_d is defined as a linear model that connects the disturbances to the outputs. When G_d is factorized into its singular values, a measure is obtained of the effect of the disturbances on the outputs.
- Closed loop disturbance gain, CLDG.
- Relative disturbance gain.

For more detailed information on interaction parameters, see Skogestad and Postlethwaite (1996).

The evaluation of the controllability performance is valuable input for the final flowsheet selection during the process synthesis (Perkins, 1989).

8.4.10. Establish the Final Pairing and Design the Controllers

This is the working platform for the control specialist. When a control strategy for a process has to be developed, the first step is to compute the RGA matrix as a function of frequency for the pre-selected pairings. The selection of the adequate set of input–output pairs is the challenge in reference to the following aspects:

- Prefer yielding the RGA matrix close to identity at frequencies around cross-over to ensure that instability is not caused by other loops.
- Avoid pairing with a negative steady-state relative gain.
- Prefer a pairing with minimal restrictions on the achievable bandwidth to obtain acceptable disturbance rejection while realizing stability.

The next steps are to:

– compute PRGA and CLDG, and plot these as functions of frequency;
– analyze potential individual loops for stability, and feasible performance bandwidth;
– avoid input constraints at frequencies where control is required; and
– select the pairing for controller design.

8.4.11. Develop and Test the Performance of the Controller in a Dynamic Simulation

The controllability analysis objective was to select pairing of CVs and MVs based on simulations to achieve robust control at the basic control layer. The controller design can start, based on the selection method. The control design can effectively be verified and tuned by implementation in the dynamic simulation. The above selection procedure does not necessarily result in a set of pairings, but still might be subject to unacceptable interaction The solution can be found in de-coupling of the loops by defining the relation of the interaction derived from the fundamental models. The interaction is neutralized in a multi-variable controller at basic control level as presented in the next section.

8.4.12. Model-based Control at the Basic Control Level

Model-based control has a reflection of a complex multi-variable controllers which have predictive, optimizing, and constraint control properties. These are quite commonly designed based on input and output modeling, but are less reliable and require ongoing maintenance. These impressions are valid, and mainly caused by the limited validity of the models. The modeling errors can be found in the process, its constraints, and its predictions. Despite these limitations, they have found wide acceptance for predictive and constraint control, and have obtained a solid position in the operational pyramid (see Figure 8.1).

The above does not limit the model-based control layer from performing some elementary calculations to support control, without compromising on robustness.

Model-based control at the basic control layer must be restricted in order to achieve the required level of robustness. These restrictions within the current state of the technology are:

- Apply algebraic equations which make solving a straightforward exercise.
- Avoid optimization and iterations – a straightforward answer is not guaranteed.
- Avoid constraint control – constraints are always difficult to model.
- Avoid predictive action, as these introduce a level of uncertainty

The models are preferably derived from fundamental models, including mass and energy balances which have a wide application area.

With the above restrictions in mind, there are still many opportunities for applications. The applications of ratio controller or feed-forward controller provided with corrections for response times are the most elementary. The design of a controller based on heat balances (as applied in Figure 4.29 in **Chapter 4**) is a simple example. A more pronounced application of the development of model-based control at the basic control layer is published by Verwijs (2001) and is described below.

An exothermal hydrogenation plug flow reactor designed as a tray bubble column (illustrated in Figure 8.18). The reaction is performed in a slurry type co-current, up-

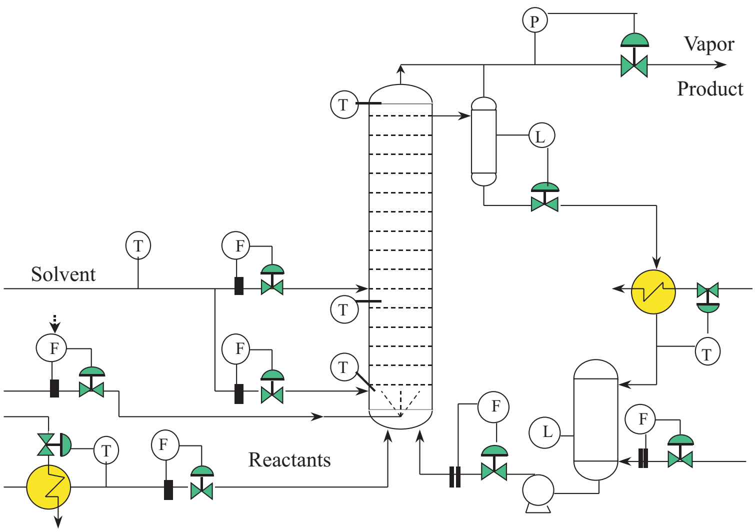

Fig. 8.18. Initial reactor control design with operators to control six interactive loops (Ref. Verwijs '01).

flow reactor which contains the finely suspended catalyst, while the heat is removed by evaporation of the product. The reaction (which proceeds to extension) takes place at the liquid–solid (catalyst) interface. Due to the large heat of reaction, a solvent is introduced at the feed point to flatten the temperature profile, and the solvent is also removed in the vapor phase. The solvent is split and supplied as quench stream at two places in the column. The control of the temperature over the reactor is critical as it determines the conversion which must go to completion while it is constrained by a run-away reaction which will develop at higher temperatures. The temperature profile goes to a peak value at one third of the height, where it is quenched with the solvent.

The system is pressure-controlled at a fixed setting. The control system as originally designed with flow rate controllers for the reactants which required adjustment during start-up and shut-down. Apart from the criticality of the control of temperature profile, the liquid hold-up was critical. Any deviation in the heat balance of the system results in accumulation of liquid in the reactor, with potential boil-over or drying out of the top part of the system. This would lead to too low a conversion and interruption of the catalyst recycle. The physical phenomenon which impacts the reaction is the gas/liquid flows in the reactor. The gas and liquid flows determine the hold-up on the trays (which is very sensitive to these flows), while the flow regimes also change upward in the column due to the volumetric changes of the gas and liquid flows. The hold-up impacts the conversion of reaction.

The whole system was in hands of the operators, who had six basic loops available: feed and solvent flow rates; ratio controller; pressure and level controllers. There was no feed-back controller for conversion/temperature profile control, heat balance compensation to keep hold-up in the system. Neither was there any type of coupling for capacity ramping. The operator had multiple set points of basic loops available for manipulation, all of which had a high level of interaction. A trip system was available to cope with temperature excursions. Thus, the operator had a difficult task to operate the system at design conditions, as any upset would cause an off-spec product as a result of too low conversion.

The challenge was to develop a control design to unload the operator with capacity control to ramp the process up, and provide feed-back controllers for conversion through temperature profile control and energy balance control by liquid hold-up regulation. The control design was planned to be executed at basic control level, and did not include any predictive or constraint controller. The design started with the development of a dynamic reactor model. The kinetics and overall conversion rates were collected from the literature, while physical properties were obtained from public data banks. The reaction kinetics had to be implemented in a tray reactor model, and were described in stages. The tray model had to include hold-up calculations which were subject to gas and liquid flows and heat and mass transfer terms. The model was written in gPROMS (Process Systems Enterprises).

The model was verified at basic reactor conditions. This was also accepted as the nominal operation point with regard to conversion and peak temperature level and location. These last conditions were constrained by safety aspects and the physical system.

The capacity set points for ramp-up conditions were calculated for reactants and solvent flows as well as the inlet reactor temperature values over the projected capacity range at design conditions. These results were converted in polynomial correlations for the feed-forward flow controller.

Heat balance control was realized by fine adjustment of the total solvent flow with a feed-back signal from the level of the catalyst recycle drum.

Reactor temperature profile control. The catalyst flow was kept constant. The profile was primarily reflected in the peak temperature, which was influenced by the overall solvent flow and the split of the solvent flows. A feed-back loop was installed between the peak temperature and the solvent flow and its split.

All the above controllers were installed in the basic control layer, and resulted in robust control of the system, while the operators were no longer part of the control loop (Figure 8.19). The whole control design was based on fundamental models, which were also used to test and tune the controllers.

The above illustrates how, based on fundamental dynamic models, robust control design can be developed for interactive process systems. The selection of the feed-back loops was based on: de-coupling of capacity control, heat balance control and conversion control through the temperature profile. The control design was implemented at basic control level based on simple algebraic equations.

The example is a nice illustration how interaction between capacity ramping, energy balance and conversion control can be de-coupled.

The same models are to be used to simulate the start-up of the reactor system resulting in an operational procedure to achieve first pass prime production.

The control design effort resulted in hands-off operation of the reactor system. The improved control supported the elimination of several decanting and off-spec tanks which made the process much more complying with a simple and robust design at lower cost.

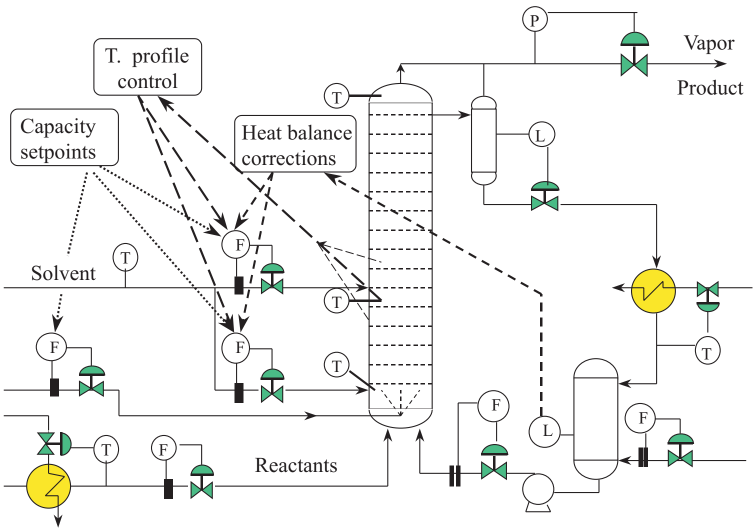

Fig. 8.19. Reactor control design with hands-off control (Verwijs, 2001).

8.5 Summary

Simple and robust process plants require robust control designs for hands-off operation. The design of robust control is an effort which requires a fundamental model-based design approach, and this is receiving an increasing amount of recognition. The robustness of the control design needs to be achieved at the basic control layer which is the fall-back control position when higher control hierarchies fail or are not available. The requirement that operators should not be part of the control loops demands quantitative process understanding to unable robust control design. Heuristic control approaches are still of value, but in time they will be superseded by fundamental control design.

A methodology for the design of basic control design based on fundamental models is discussed, and consists of the following elements:

- Dynamic model building based on fundamental models.
- Preliminary selections of CVs and MVs, measure variables and disturbance variables.
- Design of overall plant wide control layout.
- Selection of dominant control variables.
- Selection of variables based on self-optimizing control structures.
- Evaluation of loop pairings to minimize interactivity based on dynamic control parameters..
- Design of controllers which might include de-coupling algorithms based on algebraic equations.
- Testing of controllers.

The approach has been completed with a control design example of a complex interactive reactor system implemented at the basic control level. The result was a hands-off operated reactor system by de-coupling capacity ramping, energy balance and conversion control. The system simulated was to comply with first pass prime production. This approach supported the elimination of several decanting and off-spec tanks and as such contributed to a simple and robust design.

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Chapter 9
Operation Optimization

9.1
Introduction

The overall objective of a simple and robust process plant says that, "An optimal designed safe and reliable plant, operated hands-off at the most economical conditions". This statement immediately points to operation optimization (OO), and as it was formulated in the design philosophies as "operation optimization makes money". In this chapter, an historical overview is provided of developments in the field of OO, together with an introduction about closed loop optimization (CLO) in continuous processes.

The description of an on-line performance meter of the process plant is seen as a key instrument to ongoing measure plant performance. The instrument can also be used for validation of OO models and tracking the closed loop optimization (CLO) performance. The accuracy and the design of such a meter is discussed.

The functioning and the design of CLO for continuous process plants is discussed extensively with the implementation procedure.

There are two specific points to be mentioned to limit the complexity of OO. First, the concept of *self-optimizing control*, which is a recent development to operate units at the optimum. The approach is based on the evaluation and selection of control variables with constant set-points to be implemented in a simple feedback loop to operate satisfactorily (with an acceptable loss), subject to the expected disturbances. Several examples have been reported in the literature to support the concept. This approach makes the modeling less complex, and also strives for a simpler control structure by avoiding MBC, such as for dual composition control in rectifying operations.

A pragmatic approach for OO. is explained. The ultimate CLO is not always the optimal solution for OO. A qualitative approach is presented for a gradual implementation of OO up to an economic level. A step-wise approach is worked out, using the following sequence of development/implementation: reactor modeling; performance meter implementation; off-line optimization model; process stability; and quality control, including self-optimizing control, eventual followed by constraint control and CLO.

9.2
Historical Developments

OO is an activity which was introduced gradually into the process industry. It began in the 1960s and 1970s with the scheduling of batches and equipment for processing steps based on mixed integer linear programming (MILP).

Particular equipment selection optimization was developed and introduced at an early stage for the large mechanical workshops, where the production was often limited by the different machines that were required for the different manufacturing steps.

Based on LP techniques, production planning became also practiced. During that same time-frame, off-line optimization for crude distillation at refineries started based on LP with a Simplex optimization technique. The operation of the refineries showed a higher productivity as a result of the implementation of the calculated operational regimes for the different crude oils. These models were also applied to feedstock evaluation. The introduction of LP optimizations in the process industry started for scheduling within the typical batch processes of drug and food manufacture.

At the beginning of the 1980s, commercial modeling software became available commercially, based on non-linear programming (NLP) techniques with a sequential modeler for process simulation. The NLP techniques were very quickly accepted as tools for process design, particular for the chemical industry. Most of these designs are complex and non-linear. By the end of the 1980s, equation-based modelers were available for process flowsheeting. The software was specifically developed for much faster solution of very large problems, and also had the capability of handling dynamic simulation. The introduction of NLP equation-based modeling was completed with an optimizer as SQP (Successive Quadratic Programming). This was the first opening for operation optimization of non-linear continuous processes. In the meantime, the capabilities of computing systems was passing through an exponential growth curve.

The availability of these tools made it possible for them to be used initially for off-line OO in the process industry. A number of off-line optimizations were developed for those continuous process industries which were subject to varying markets and feed stock conditions. It should be mentioned, that these variations should not be too frequent (less than once a day). The models were also applicable for feed stock evaluations. Refineries also converted their LP optimization into NLP optimizations, to achieve a higher accuracy level, and this resulted in more savings and extended the applications to other units such as hydro-crackers (Marlin and Hrymak, 1997).

A model with high accuracy makes it possible to operate closer to the plant constraints. Savings, reported by different companies, all showed that productivity improvements were in the order of percentages of the operational cost for plants, subject to variations. Engineers from process plants that were exposed to less variable conditions learned that several plant conditions needed to be adapted significantly to comply with optimal conditions, and so achieved considerable savings.

During the early 1990s, several complementary developments also took place:

- Computing power was increasing exponentially, and was no longer seen as a constraint.
- Model-based controls such as predictive constraint control were applied at a larger scale in the process industry, the refineries being the leaders in this field.
- First applications of CLO based on NLP were introduced in refineries as well as ethylene plants.
- The first commercial executive systems for CLO were installed.
- The optimizers could solve very large problems as LS-SQP (large-scale successive quadratic programming)

During the 1990s, computing power developed so rapidly that it was no longer seen as a constraint on OO, which has been implemented in several large chemical plants next to olefin plants (Factora et al., 1992), at hydrogen, benzene, ammonia, nitric acid, ethylene oxide plants.

The technology is still very young, and the practical applications are mainly limited to steady-state conditions. Future developments will include dynamic optimization to be used for optimization of: transient operations, gradually fouling systems, and dynamic optimization of continuous fed-batch reactor systems. Transient operations often taken place in continuous polymer plants that change from operational conditions to produce other grades. The amount of transient material, which has a lower product quality and value, can be minimized by the application of an optimal change over. The optimization in fouling systems such as catalyst aging or coke formation is another field for optimization. In these situations, the run length between cleaning or regeneration and the operational conditions over the run length are subject to optimization. Dynamic optimization of batch reactor systems can increase reactor capacity and product quality. The developments that are required in order to implement these at commercial scale include:

- Accurate dynamic reactor and fouling models for the specific systems.
- Dynamic optimization techniques in a commercial format.
- Nonlinear model-based controllers.
- Accurate on-line measuring techniques for product properties with short response times, particular optical techniques are full filling this opportunity.
- On-line model validation techniques.

These developments are already under progress within the academic world, but need to be proven at plant scale.

9.3
General Operation Optimization of Continuous Processes

9.3.1
Incentive

The objective is to operate a process plant on-going at its most economical conditions. This can only be realized if operational conditions are evaluated and implemented each time the surrounding conditions are changed. The following circumstantial conditions will impact on economical performance:

- Price changes of raw materials, products, energy.
- Feedstock changes.
- Production capacity.
- Product quality.
- Meteorological conditions (may restrict capacity and pressure operations).
- Process parameters as fouling, aging, catalyst quality.
- Transient operation.

The spin-off of OO can be considerable. The development of an OO package in whatever form always drives a process unit to its constraints, or into the edges of its constraints. This forces the developers and operational personnel to build up an extensive knowledge of the process constraints. The knowledge of these constraints, which limit the operational capacity, may trigger engineers for relative simple hardware modifications to achieve cheap capacity increments.

OO is critical for the economic operation of the facility and its relation to other plants and the overall business. The prices used for the raw materials, products and energy are crucial for the optimal operation. The economics of OO are normally based on incremental conditions. Due to the criticality of the issues mentioned, it is essential to involve an economic evaluator from the business to achieve agreement about:

– objective function;
– economic calculations as incorporated in the optimization routine; and
– prices and their regular updating.

Most of the circumstantial conditions change at a certain point in time, and remain constant for a while (prices, product quality), while others are subject to continuous change, for example meteorological conditions.

9.3.2
Continuous Processes

These are normally operated around a steady-state point. The optimization calculation procedure is based on a process model and represented in a control loop (Figure 9.1). The consequence is that every time conditions change, the steady-state situation has to be updated. The frequency of the changing conditions determines if the operational adjustments will be implemented manually or automatically.

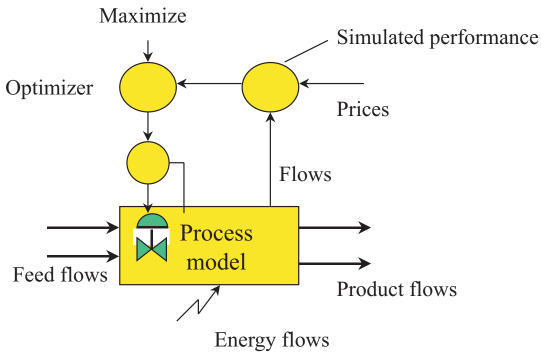

Fig. 9.1. Process oprimization reflected in a control diagram.

Manual implementation of adapted process conditions is executed based on off-line optimization results. Manual updating is normally done on a daily basis, or at any significant change such as processing of another feed as crude in a refinery. The number of degrees of freedom (DOF) in general is limited in an off-line optimization. During the implementation of off-line optimization conditions, the process is normally not running close to its constraints, unless constraint controllers are installed. Operators prefer to stay away from constraints to avoid all kinds of interacting actions

Automatic implementation of process conditions is based on continuously running optimizations, which receive ongoing updated circumstantial information; this is called CLO. Operational conditions are however only changed in discrete steps. The discrete implementation steps are the result of: the time it takes to execute an optimization cycle; and the variation of the circumstantial conditions which often is based on information which becomes available at discrete times, for example price sets.

OO as a whole needs to be seen in a hierarchical control structure, as reflected in Figure 8.1 in **Chapter 8**. As a basis, there must be DOF available for manipulation, to achieve a more economic operation.

A CLO cycle must follow a stepped sequence that is enforced through an executive (Figure 9.2). The sequential steps are:

- data analysis;
- data reconciliation;
- parameter estimation;
- optimization; and
- implementation of new set-points.

Before a step is terminated and the next step is activated, a set of decision criteria must be met. The individual steps will be described in detail in the following paragraphs.

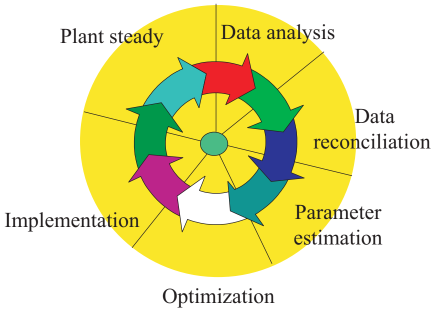

Fig. 9.2. Optimization cycle.

Savings to be realized can be divided into operational cost savings and capacity increments.

Operational savings are realized by: higher selectivity; fewer lower-value products; lower energy consumption; and less waste or off-grade material.

Capacity increments (higher capacity) can result from better scheduling, shorter runtimes for batch plants, shorter product change-over times, and constraint control on capacity limiting units. Many continuous plants have units that are limited in capacity by environmental conditions such as:

– Heat exchangers cooled by cooling water or refrigeration (refrigeration is often limited by the condenser of the cooling medium).
– Air coolers.
– Air blower that set the capacity for furnaces.
– Air compressors that determine the power output for an gas-turbine.

These processes have the option to take advantage of the day and night temperature cycle by adapting the process capacity over the 24-hour cycle (Figure 9.3). Capacity increments of 5% are achievable by exploiting this option.

As an order of magnitude, the operational savings can be up to 3–10% of the variable operational cost, while the capacity creep will reach up to 5–10%. The higher saving levels are only realized if more optimization activities are implemented, such as scheduling and shorter run-times for batch plants or optimization of transient operations in addition to constraint control on capacity operations. These savings are based on industrial data. It should be understood that these savings reflect the overall saving as a result of improved control, as well as improvements made by optimization. It will be obvious that the savings must be determined for each specific situation, and this will be discussed in more detail under Feasibility studies (Section 9.6.1) (White, 1999).

A more structural prediction method was developed by Hennin et al. (1994) and Loeblein et al. (1996), as will be mentioned under feasibility studies.

The *level of accuracy* of OO is an important factor. It was said earlier that the contribution of OO is in the order of percentages of the operational cost. The conclusion might be justified that in this perspective, an OO needs to have an accuracy of at

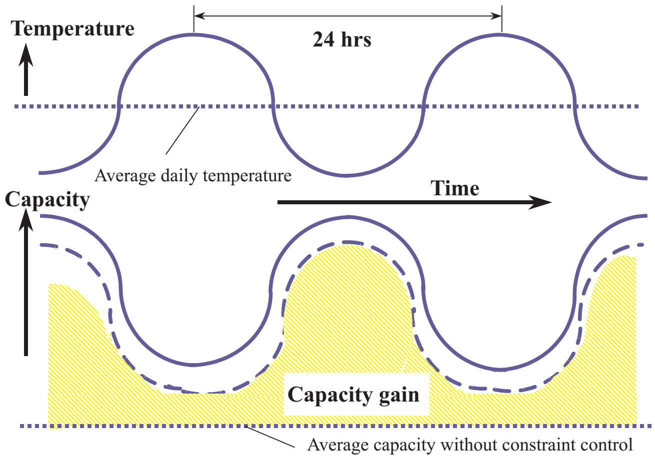

Fig. 9.3. Effect of the day and night cycle on capacity.

least 10–20% of its projected contribution; this means on the order of tenths of a percent of the operational cost. It is important to realize that:

Any inaccuracy of an optimization activity results in a missed opportunity.

The challenge to achieve this high level of accuracy is often under-estimated. At the same time, the ultimate contribution of the operational cost reductions are often not measured. This in contradiction with the capacity performance, which can be obtained from the capacity performance measurement and often receives much attention (see also **Chapter 10**, Section 10.2.1.)

Validation of the optimization activities up to the intended accuracy is not a trivial task. The factors that play a role in the achievement of this task are:

- Accurate model description, including constraints.
- Parameter estimation (updating on line).
- Steady-state operation for validation of the model, as well as for implementation in a quasi steady-state process.
- Validation technique based on the minimization of deviations.
- An on-line overall performance measurement.

9.4 Performance (Profit) Meter

In order to quantify the required level of accuracy of optimization, the process must be provided with an on-line performance measurement (Krist et al., 1994; US Patent 6.038,505). The meter calculates the performance of the process in money terms per unit of time. The performance meter is based on an accurate reconciled mass balance/heat balance over the process and convoluted with the related prices of the individual streams, and calculates the ongoing actual performance of the process. The mass and heat balances were chosen as these are based on the conservation laws which do not require model validation.

Mass and energy balance reconciliation techniques are extensively applied by plant information systems (e.g., OSI Software, MDC and Vali II software), but also can be configured within the software used for on-line optimization. Several applications of reconciliation and model validation were reported in the Vali user group meetings of Belsim.

The performance measurement is expressed as the variable operating margin, and does not include any capital-related term cost as interest or depreciation; neither does it include any manpower costs and maintenance costs.

The variable operating margin **M** is defined as:

M = (Output-Input) per unit of time expressed in money units per unit of time (t)

M = Product revenues / t – Feed (raw) material cost / t – Energy cost / t

$$M = \Sigma\,[\Sigma_i\,\pi_i\,P_i - \Sigma_j\,\varphi_j\,F_j - \Sigma_k\,\varepsilon_k\,E_k - \Sigma_l\,\alpha_l\,\Delta A_l] \qquad (1)$$

where P = Product flows, F = Feed (raw) material flows, E = Energy flows, Δ A = difference in Accumulation. P, F, E, A in unit mass/energy per unit time.

π = product prices, φ = raw material prices, ε = energy prices, α = material accumulation price. π, φ, ε, α in money units per unit mass/energy, and t is time.

The performance meter is illustrated diagrammatically in Figure 9.4.

The continuous performance measurement can be utilized for:

- Ultimate validation of an optimization model by comparing the simulated performance versus measured performance. The difference needs to be minimized and at least within the required accuracy over the operational range of the process.

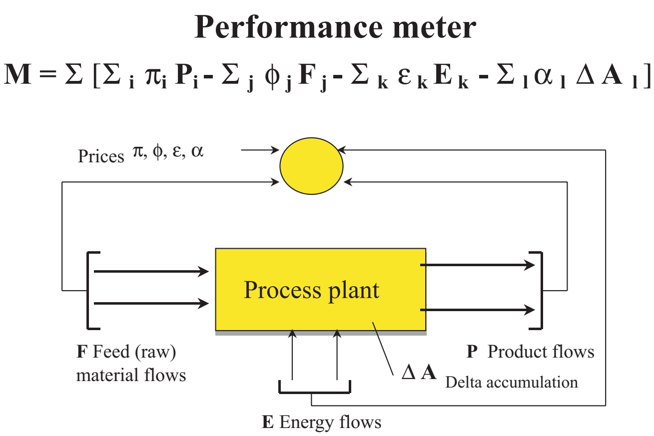

Fig. 9.4. Perfomance or profit meter.

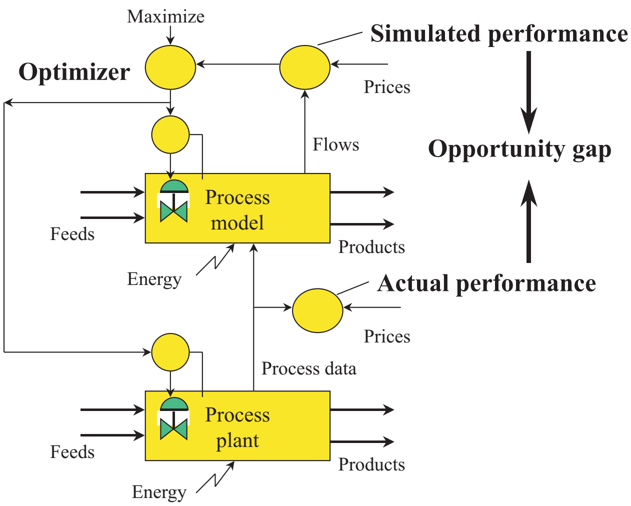

Fig. 9.5. Measurement of actual versus simulated performance.

- Validation of the contribution of hardware as well as software projects (control or optimization projects) on their contribution. To facilitate this, the performance measurement can be run with fixed prices, but must be installed before the implementation of these projects.
- On-line communication of performance for operation and business to provide feed-back on operational/business actions.

The measurement of actual performance of the plant in relation to the simulated performance of the optimization is reflected in Figure 9.5. The challenge for the developers is to minimize the opportunity gap through validation and correct updating of the process models.

9.4.1 Design of the Performance Meter

The design of a performance meter is based on the reconciliation of mass and energy balances of a process over a time interval. The process may include process sections as well as storage, while the time interval selected depends on the application. The performance can be measured on a continuous basis and accumulated over a time period; this can also be applied to continuous plants. For batch plants, the performance might be measured per batch/recipe. For continuous plants with transient operations to produce different products, the functionality might be a mixture of these.

It was said earlier that the accuracy of a performance meter is essential for its function. Such accuracy is determined by the mass balance reconciliation in which three factors play a role:

1. Measurement accuracy
2. Degree of redundancy of the flowsheet
3. Process variability

9.4.1.1 **Measurement accuracy**

This is initially determined by the selected instrument. It is common practice to measure the volumetric flow and to calculate the mass flow based on an assumed density, but this already introduces a considerable error. Most streams are subject to density variations caused by temperature or concentration, while the density is often not measured together with the volumetric measurement. In addition, there is also a volumetric measurement, such as an orifice, that is already density dependent. In this application a mass flow meter is recommended, not only to avoid these implicit errors, but also to create a high accuracy.

9.4.1.2 **Degree of redundancy**

This is achieved by installation of additional measurements for reconciliation of the flowsheet. An example of adding redundancy is shown in Figure 9.9. The addition of more redundant nodes is illustrated, in the bottom part also the storage area is included in the flowsheet. The accuracy of the individual streams can be calculated for the selected flowsheet based on the installed instrument accuracy. and described in the Appendix 9.1 (Heyen, 1994). This has been extended by Heyen et al. (1996) by the introduction of the contribution of the variance of measurement k in the estimation of the variance of reconciled state variable i. These contributions might be listed in order of impact. Conclusions drawn in this leading article, about these sensitivity analysis are:

- Which are the measurements that contribute significantly to the variance of the validated results for a set of state variables?
- Which are the state variables whose variance is influenced significantly by the accuracy of a given measurement?
- How is the value of a state variable influenced by the value and the standard deviation of all measurements?

The sensitivity analysis has been implemented in Vali II software from Belsim.

9.4.1.3 **Process variability**

Depending on the application of the performance meter, the process dynamics play a role in the performance measurement. There are different ways to limit the effect of process variability:

– Integrate the measurement over a larger time interval.
– Include process hold-up variations in the model.
– Improve process stability.

If the results are integrated over a longer time period, the variations in hold up within the process will have a reduced effect. If storage is included in the flowsheet, the variations in storage are considered to be captured in the model.

Hold-up variations in the process might be included in the flowsheet model by defining a vessel with hold-up measurements (level).

Process stability has a direct impact on performance meters with a relative short integration time, as used for CLOs. The only way to achieve this is through improved control. This would make it possible to narrow down the criteria for steady-state detection and so would impact on the calculated value over smaller time intervals. The noise of the signal (performance) would be reduced and as such make it a more accurate measurement for tracking of CLOs.

The model is mostly written in the same simulator (equation-based with open equations) as the process model and the design of the performance meter is combined with the data reconciliation step. A stand-alone performance meter is designed to be simpler in which case the optimization routine is written explicitly to avoid installing an extended simulator/optimization package.

Summary

In general, operation optimization of continuous processes include:

- The objectives for process plants are to operate continuously at the most economical conditions in a continuously changing environment of: feed product and energy prices, capacity, feed compositions, product qualities and distribution, aging/fouling factors of process equipment and catalyst, meteorological conditions, and transient operations.
- OO might be executed off-line versus closed loop; off-line optimization is preferred when the conditions for the plant do not change frequently (daily basis), while the number of DOF is limited.
- CLO follows a sequential operational cycle to be discussed in detail in the next section.
- OO savings to be realized are in the order of percentages of the variable operational margin, while capacity increments may fall in the 5–10% category.
- The level of accuracy required for OO models is rather high, in the order of tenths of a percentage of the operational cost. The following statement supports this:

Any inaccuracy of an optimization activity results in a missed opportunity

The validation of OO models to achieve the required accuracy next to model building is a very conscious activity.

- Performance measurement is a detection method to measure the variable operating margin of an on-line process based on reconciled mass and heat balances and prices. The measurement is designed continuously to track the performance of a process, and can be used to detect mismatch between actual and simulated performance; thus it is an ultimate validation of the simulation. The design of an accurate performance meter is discussed.

9.5
Closed Loop Steady-state Optimization

In this section we will discuss different OO techniques and the basic modules for the execution of an optimization cycle for continuous (steady-state) and dynamic operations (Krist et al., 1994; van Wijk et al., 1992; Marlin and Hrymak, 1997; US Patent 5,486,995; US Patent 6,038,540). During this discussion we will illuminate the different technical aspects around process optimization. Off-line optimization is not discussed separately, but most of the elements discussed are also applicable in that specific situation.

9.5.1
Optimization Techniques

Three different operation optimization techniques can be recognized for a continuous process plant, and these are discussed prior to the modules of the optimization cycle:

1. Self-optimizing control/optimized unit control
2. Empirical optimization
3. Fundamental model-based optimization

9.5.1.1 Self-optimizing control or optimized unit control

Self-optimizing control is a technique developed at the University of Trondheim, Norway (Halvorsen and Skogestad, 1997, 1999; Skogestad, 1999, 2000; Skogestad et al., 1998, 1999).

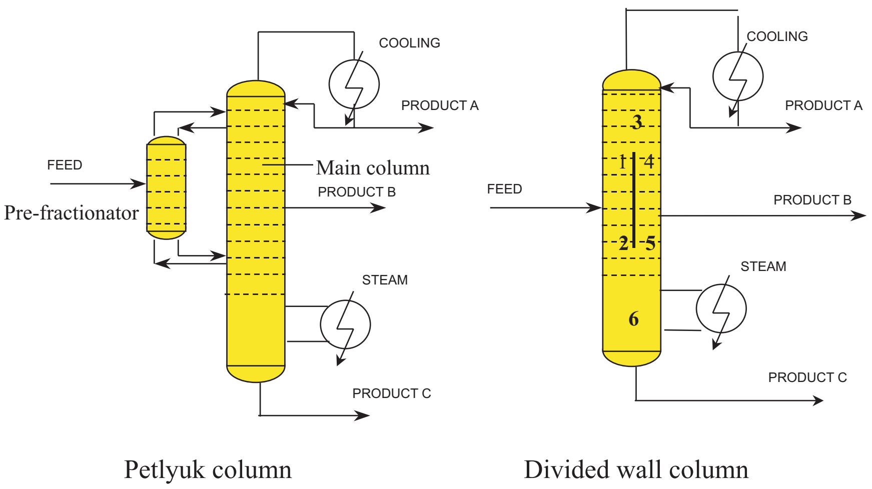

Fig. 9.6. Petlyuk column and divided wall column both capable to separate a three component mixture at required specification.

The technique is applicable to process systems/units that have more degrees of freedom available than output specifications, and the optimal solution of a suitable criterion function is unconstrained. The work was evaluated for an integrated Petlyuk distillation column (Petlyuk et al., 1965). The Petlyuk column, which in a more practical form was presented by Kaibel (1987) as a divided wall column (DWC), is a distillation column that separates three products at required purity (Figure 9.6). A DWC has a lower capital investment as well as lower energy cost, up and to 30% compared to conventional distillation in two successive columns, (Figure 5.7 in **Chapter 5)**, (Triantafyllou and Smith, 1992). The DWC is an excellent example of simple and robust design, less equipment and related less capital, less energy consumption and as such a lower cost of operation.

The self-optimizing control study was carried out for a DWC where the top and bottom qualities were controlled, as well as the quality of the side stream, with regard to one impurity. Previous studies have shown that such a column does not necessarily have strong interactions for the control of product qualities. Optimization of the DWC showed the optimum of such a column to be very sharp (Halvorsen and Skogestad, 1997). During the early investigations, researchers considered that the optimal operation point of such a column would be difficult to maintain in case of disturbances. However, this was questioned by Halvorsen and Skogestad (1999), who subsequently evaluated a self-optimizing control for this application. The two manipulated variables (DOF) available for optimization (not utilized for control) were the liquid and vapor split between both separated parts of the column (prefractionator and main column). The objective of the optimization for this application was translated as, minimization of the energy stream to the reboiler, translated in vapor flow V. In a self-optimizing control, the key is to determine the effect of disturbances on the optimal operation point, and to find a common measurable variable with a near-constant value at these optimal conditions. In case such variable can be found, a control loop can be implemented based on a simple feedback controller. The disturbances (*d*) studied were: feed flow rate, feed composition, feed liquid fraction, and product purities The choice was made to select the liquid split (*u*) as the only manipulated variable, and to fix the vapor split. Eight feedback variables were selected for evaluation. The optimal solution was found by minimizing V (*u, d*) with respect to *u*. The optimal value of the criterion function V_{opt} and the corresponding solution u_{opt} will be a function of d

$$V_{opt}\,(d) = \min_{u} V(u,d) = V\,(u_{opt}\,(d),d \qquad (2)$$

The methodology was evaluated for a chosen system. The boil-up V and the liquid split u (at a fixed vapor split) with self-optimizing control for different feedback cases for the selected disturbances were compared to the overall optimal boil-up values. The overall conclusion was that self-optimizing control was a good method for optimization of a Petlyuk column. The selection of the final feedback variable depends on the most probable disturbances, but three of these were selected as the best with errors within 1%. The three selected feed back variables were:

1. Fractional recovery of the intermediate component B leaving the pre-fractionator top.
2. Fractional net recovery of the bottom component C in the overhead of the pre-fractionator versus the total net flow of C to the main column.
3. DTS – a measure of temperature profile symmetry,

$$DTS = \sum (T_{1,\,i} - T_{4,\,i}) + \sum (T_{2,\,i} - T_{5,\,i}) \quad (3)$$

where $T_{N\,i}$ is the temperature of tray i of section N, for the temperature location (see Figure 9.6).

The last mentioned feed back variable can easily be measured by temperature, while the others require a composition measurement.

The above self-optimizing technology can be seen as a suboptimization of a global optimization problem (Figure 9.7), or as part of the control layer. The global optimization sets the feed composition (direct or indirect), next to the product specifications. The self-optimization reacts to any disturbance to keep the unit at its optimum energy consumption. In the case of final products, the purities are often firm constraints, while recycle streams often have economic specifications that are subject to change and need to be updated by global optimization.

The search for self-optimizing control structures is discussed by Skogestad (1999) in a more generic paper that is illustrated with some other examples as a reactor system and a simple distillation column. For a further description, see **Chapter 8.** In

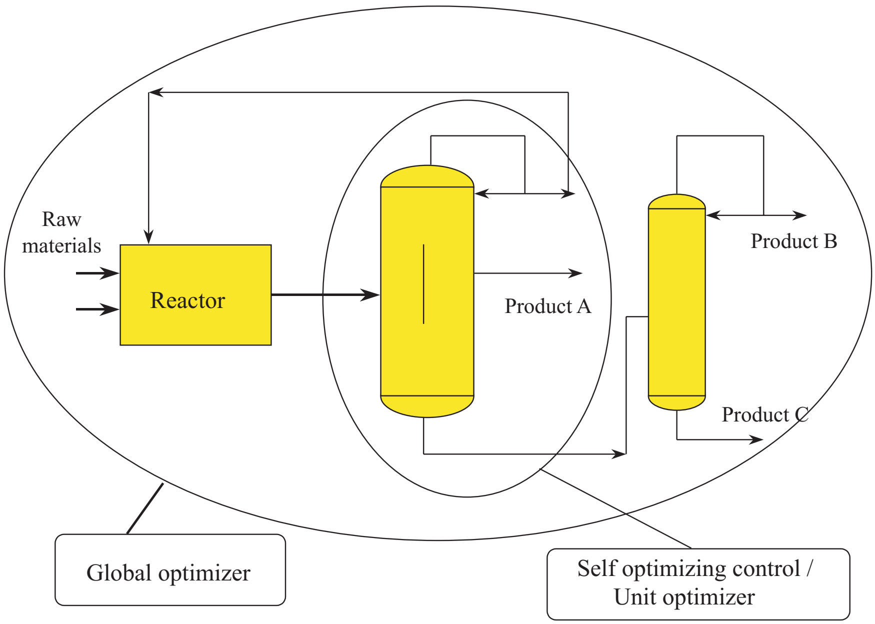

Fig. 9.7. Global optimization versus unit self optimizing control.

Skogestad's paper, self-optimizing control is defined as: "... when we can achieve an acceptable loss with constant set-point values for the controlled variables".

In these studies, a methodology was developed based on steady-state simulation to select controlled variables based on loss criteria. The idea is that local control, when based on simple feedback and with the correct variables, might take care of most disturbances. This would reduce the need for continuous optimization, or it would close the gap between the optimization cycle. The methodology calculates the steady-state losses for different control variables which were subject to disturbances. In the example of a propylene propane splitter, Skogestad demonstrated that the losses for a dual composition controller were in the same order as a controller for the top quality control and one with a constant reflux to feed ratio (L/F) or vapor feed ratio (V/F). This led him to the conclusion that a dual composition controller in this case would better be avoided due to high interaction leading to complicated model based control (MBC), which also would have additional dynamic losses.

The advantages of self-optimizing control are:

- Disturbances will immediately result in process conditions adapting to keep the system close to its optimum; there is no need to wait for the next global optimization cycle.
- Global optimization problems have a tendency to become very large in size, making it difficult to maintain the models. Self-optimizing control is a method to implement the optimization in layers, which makes the problem more surveyable.
- Selection of the correct control variable leads to simpler feedback control configurations which still operate satisfactorily (with acceptable loss)

A disadvantage are the limited losses incurred.

Wider applications for self optimizing control Self-optimizing control may be evaluated for application to several units. However, one precondition is that there are more DOFs than output specifications, and the optimal solution of a suitable criterion function is unconstrained. Applications of self-optimizing control are: dual composition control on a distillation column, but also the control of a near-total conversion hydrogenation reactor where the hydrogen supply is controlled. Another potential candidate might be an extractive distillation column in combination with a stripper.

9.5.1.2 **Empirical optimization**

Empirical optimization is an approach; this is not often applied, and in essence is a black box approach with specific limitations. The approach is based on the development of a process model on input/output analysis, as applied to the development of a model-based controller. The input/output model is generally developed on the process itself, but it also might be developed on the process model. The latter option is often not available, or at least not at the required accuracy. The development of an input output model has similarities to the development of a dynamic model for model based control. For the model development the effect of step response is measured for selected variables. The selected variables are those who might have an significant effect on the operation of the process, they include feedstocks as well as reactor conditions also environmental effects can be included.

In general, empirical optimization is limited to processes with:

- four to five DOFs for optimization;
- constant quality feed streams;
- fundamental process model not available; and
- not subject to any fouling, aging or catalyst activity effects, which would have a negative effect on the plant performance.

Processes with one reactor and a few separations based on pure components as reactants and limited conversions of one of the reactants are candidates for this approach.

For the development of the model must:

- Define the operating window of the process for optimization.
- Assign the degrees of freedom relevant for the optimization.
- Develop an experimental design program to determine the impact of the DOFs on plant performance over the whole operating window of the plant.
- Develop and implement a mass balance around the process with sufficient redundancy to enable a mass balance reconciliation (this can utilized later for the installation of a performance meter over the process; see Section 9.4). If the mass balance cannot be closed, it may be best to stop considering optimization.
- Make a heat balance over the plant to confirm the utility consumption measurements.
- Observe if the process is stable and, if necessary, adapt the control in such a way that the process is sufficiently stable to achieve a mass balance that is stable over the planned time horizon of a test. As part of this step, determine the noise on the mass balance measurement at different operating conditions.
- Start the test program and determine the impact of the DOFs at the plant mass balance and its utility consumption.
- Develop the empirical model.
- Identify the constraints under different conditions, which set the operational window.

Based on the empirical model, an optimization needs to be built. The next step will be to develop the optimization model by adding a price section and economic section, and complementing it with an optimizer. For the implementation of empirical optimization, the best approach is to follow the methodology described later in this chapter. The optimization might be applied off-line, but it still requires adequate control with quality loops closed to achieve its maximal savings. The application of empirical optimization as a stand alone application is limited but empirical models can play a significant role as a subset of a fundamental model for optimization.

9.5.1.3 Fundamental model-based optimization

Fundamental model-based optimization is the most widely used approach, its advantage being that it forces you to know the process in detail at steady-state conditions, and the dynamic behavior in case of a dynamic optimization. Crucial points for optimization models include the need to:

- Develop the model in line with the design models (life cycle modeling).
- Develop the model in an equation-based modeling environment with open equations, to achieve fast responses equipped with an optimizer. The open form simulators/optimizers are, in concept, characterized by:
- – Each equipment is modeled by equations without nested convergence loops.
- – Derivatives are calculated.
- – All variables are accessible.
- – Robust and fast solvers.
- – Self diagnostics to identify modeling errors.
- The models to be applied are:
- – A set of equations written in residual format f (X) = 0.
- – The solution of the model equations is distinct from its formulation.
- – Equipped with detailed information about its structure as:

(i) list of equations and variables;
(ii) incidence matrix which variables are in which equations;
(iii) function to return to residual values and derivatives; and
(iv) variables can be fixed or set free:

- Target for an accuracy which is relevant for the objective. To limit the size of the problem, short-cut approaches might be used for those units that play neither an essential nor a constrained role in the optimization. Examples for simplification are:
- – the use of splitter boxes for units where energy or solvent consumption are calculated from the inlet stream,
- – short cut simulation for distillation, extraction, stripping absorption
- – lumping of trays for columns,
- – elimination of small equipment as pumps
- As optimization always means that the process runs against constraints, a detailed description is required in those areas. A feedback on process parameters which are subject to change, such as fouling of heat exchangers, compressor efficiencies, or aging catalyst, are essential when these have a relevant impact on the performance.
- Reactor models are, in general, essential for the optimal operation due to the trade-offs between conversion, selectivities, product distribution, and its aging effect. Exceptions might be reactors running at 100% conversion with a self-optimizing control on the selectivity. Reactor models might be implemented as empirical models within a fundamental-based flowsheet model. The model can be developed based on input and output analysis, although it should cover the full operational range for the optimization. The operational range is often larger than originally anticipated for a process without an optimization.

Fundamental-based models are mostly a mixture of detailed described process sections, short-cut described part based on fundamentals, and empirical models. However, it should be noted that the more fundamental the bases for the models, the higher the value of the models for understanding and upgrading the process.

The fundamental as well as the empirical approaches for optimization are both embedded in a framework for execution of the optimization cycle.

9.5.2
The Optimization Cycle

The optimization cycle, which is operated by an executive to manage the implementation of CLO, is composed out of the following sequential steps, called modules (see Figure 9.2):

- Data analysis
- Data reconciliation
- Simultaneous data reconciliation and parameter estimation
- Optimization
- Implementation

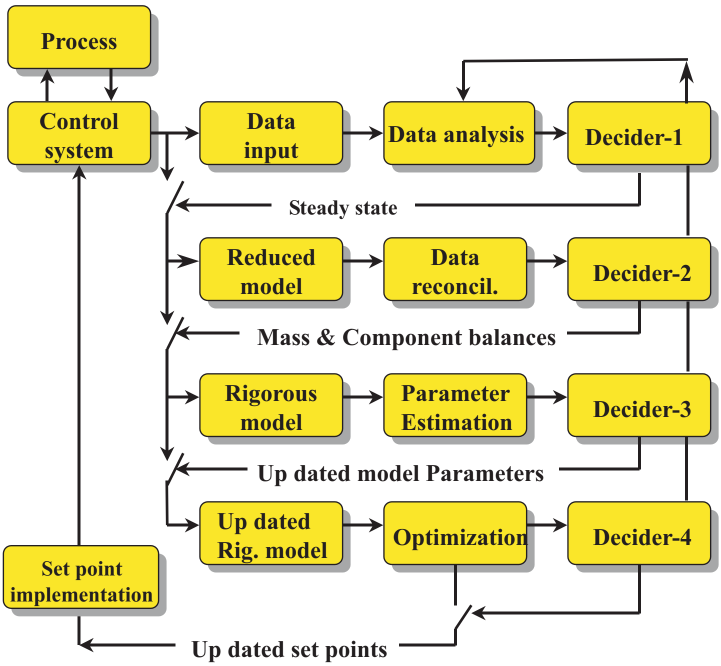

Fig. 9.8. System architecture for closed loop optimization, J. Krist et al., 1994.

The system's architecture is shown in detail in Figure 9.8, including all the elements. The description is written for a steady-state optimization. The modules, which are always complemented with a decider, will be described in sequence.

9.5.2.1 **Data analysis (DA) (Jordache and Narasimham, 1999)**

In this module, all plant data necessary for the optimization are retrieved from the basic control system, to be completed with status data from the model-based control platform. These data are analyzed for corruptness and used for the determination of process condition, and completed with a decider before transfer to the next sequential module. The data required are:

- Status data, to reflect (digital information):
- – operational state of the plants (is it in an operational optimization step?).
- – operational state of the model-based control platform (is it active?).
- – operational state of the control loops (are loops closed and available for implementation of downloaded optimal set-points? – these are the DOFs for the optimization).
- – data analysis requested, set by a timer in the executive.
- Process operational conditions for (analog information):
- – Steady-state Representing Values (SRVs) for the selection of SRVs, see Section 9.6.5. (see Krist et al., 1994 for steady-state detection);
- – Data reconciliation.
- – Parameter estimation and optimization.
- – Feed and environmental conditions, such as outside temperature.
- – Constraint conditions, such as maximum operational pressures and temperatures, speed, environmental loads.

The first task of the data analysis module is to check the existence of any corrupt data; no signals, or out of a defined range, the first pass on gross error detection by signal analysis. Gross errors in measurements are detected at different levels:

- Instrument level by signal analysis.
- BC (Basic control) level by comparison of redundant measurements such as tank levels.
- OO level by data reconciliation and parameter estimation criteria and the determination of outliers compared to simulation results.

These gross errors are selected based on decision criteria which depend on the specifics of the measurement and the process. Gross errors detection during data reconciliation are described in Section 9.5.2.2.

The second task is to measure steady-state condition. The detection of steady state is not limited to systems planned to operate as such. They may also apply to dynamic optimizations to measure process parameters that have an impact on performance, such as the aging or fouling conditions; transient operations often also start from a steady-state condition. In fouling or aging systems the dynamic optimizations implement gradually a new set-point over a long time period, and in fact move in discrete steps from one steady-state condition to the next within an optimized transient. In the case of rapid dynamic effects, steady-state detection is not applicable.

Several methods are applied to steady-state detection, including:

- mean value of a given set of measurements over a defined time period are within a certain tolerance.
- rate of change of a variable over a time period.
- constancy of time series coefficients.

An example of a steady-state detector is the application of exponential smoothing filters which in a digitized form is represented as

$$X_{f\,i} = F_l . X_i + (1 - F_l)\, X_{f\,i-1} \tag{4}$$

$X_{f\,i}$ is calculated filtered value for history i
$X_{f\,i-1}$ is filtered value calculated for the previous history (i–1)
X_i is raw unfiltered history value i
F_l is filter factor

Measurements signals have high-frequency and low-frequency noise. The high-frequency noise ("white noise") is caused by the instrument, while the low-frequency noise is caused by process noise. It is the process noise in which we have an interest for steady-state detection.

The process noise is calculated by subtracting a heavy filtered signal (absorbs high-frequency and low-frequency noise) from a low filtered signal (high-frequency noise):

Process noise = heavy filtered noise – low filtered noise.

A tolerance will be set at the process noise over a number of values in history. If the tolerance is superseded, the process is unsteady.

The criteria for steady state should not be too strict so as to avoid there being only a few opportunities left to perform a CLO.

The final task is to define the criteria for decider 1:

- Is the process still in its operational optimization step?
- Is the process meeting the steady state criteria?
- Are the corrupt measurements excluded?

The overall decision is to proceed to the next sequential step "yes" or "no", based on defined criteria. Another decision is to exclude incorrect measurement data.

9.5.2.2 **Data reconciliation (DR) (Jordache and Narasimham, 1999; Kane, 1999)**

CLO projects apply different methods to achieve a close agreement between simulated and actual operation. The objective of this module in its reduced approach is to:

- estimate the feed and its composition by the process system;
- detect any gross errors in measurements involved the reduced model; and
- measure the actual plant performance in terms of money.

Model Input data reconciliation is based on mass or mass and energy balance reconciliation. These balances have been selected because they do require any validation while based on conservation laws. The overall mass balance of the system is used to provide the simulation/optimization of the process with good input data. Feed quantity and quality are particularly important. The accuracy of the reconciliation step improves if more redundant nodes are built into the flowsheet (Figure 9.9). It might be beneficial for the increase in redundancy of the flow-sheet for the plant mass balance to include the storage area. Due to its inventory measurement, an additional redundancy is added by averaging the mass measurement over a time period. Large-sized vessels in the process can also be equipped with a hold-up measurement and taken into account for the mass balance reconciliation.

The accuracy for the reconciled data depends on: the accuracy of the individual measurements; the redundancy built into the flowsheet; and process stability. The method of mass balance reconciliation over the process is also applied to the performance measurement, as discussed under performance meter (see Section 9.4).

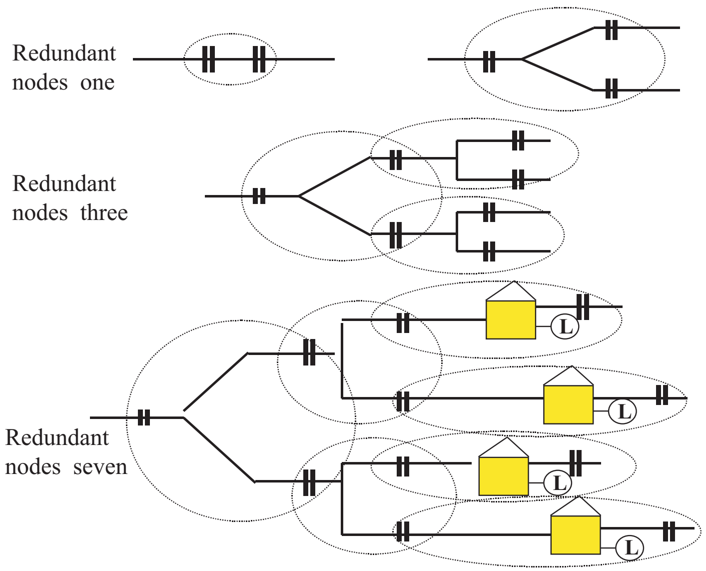

Fig. 9.9. Illustration of adding redundancy for flow measurements.

Data reconciliation technique (Britt and Luecke, 1973; Albers, 1999) This technique is based on minimization of the deviations of the square of the difference between the reconciled value of the measurement and the measured value. In formulae form:

$$\text{Min} \sum_i \left[\frac{y_i^* - y_i}{\sigma_i}\right]^2 \quad (5)$$

Subject to $F(y_i^*) = 0$

Where y_i^* is the reconciled value of measurement i,
y_i is the measured value of measurement i,
σ_i is the standard deviation of i, or confidence interval
$F(y_i^*) = 0$ corresponds to the process constraints

The equation is solved by the Lagrange multipliers method (see Appendix 9.1). The equations are solved either through minimization of the Lagrangian, or the entire set of equations is solved involving the algebraic equations obtained through partial differentiation, as well as yielding correction variables at which the Lagrangian's minimal is located. In essence, there is no difference in technique between data reconciliation and parameter estimation – in both cases redundant measurements are required to be emphasized in a model, and solved to minimize the errors.

A gross error detection method has been developed by Tamhane and Mah (1985). By definition, a gross error occurs when the error exceeds its outer limit; if not, the error is said to be random. After reconciliation, the Z statistic is calculated and defined as

$Z = (y_i - \mu)/\sigma$ (6)

where μ is the average of process variable measurement.

Z is calculated for each measured variable, if any variable exceeds a limit value Z a gross error is identified, in that case the variable with the largest Z is treated as unmeasured and the data reconciliation is repeated. If the Z of all measured variables are accepted, the reconciliation is accepted as "true". The limit is defined as the allowable absolute ratio of the error and the standard deviation of the measurement.

The significance level might be adjusted for the number of measurements by,

$$\alpha = 0.5\,[1 - (1 - \alpha)^{1/n}] \quad (7)$$

where α is the significance level.

The limit practiced by Krist was 1.96 times the standard deviation of the measurement.

After the data reconciliation step, we have a reconciled mass and component balance and a set of measurements identified with gross errors.

It is interesting to note the spread of the performance meter in money terms. If the spread is relative large, say 0.5% of the conversion energy versus an objective of a few tenths of one percent, an analysis of the causes is required.

The spread is caused by the same elements as mentioned under the design of the performance meter:

- Measurement accuracy
- Redundancy in measurements of the flowsheet
- Stability of the process

The output of the reconciliation module is a set of reconciled data to be used as actual input for the simulation.

Decider 2 Before the next step is activated, the following decisions need to be made:

1. Is decider 1 true?
2. Are the reconciled data available and within a certain pre-defined range?
3. Are gross errors removed from the data set?

9.5.2.3 Data reconciliation and parameter estimation (DR&PE)

The DR&PE module is built to achieve a close match between the operational plant and the simulated process plant. The objective of the step is to provide an updated model for optimization by estimation of the assigned parameters. The detailed activities are:

– all involved measurements are evaluated on gross errors;
– parameters estimated /calculated at actual process conditions;
– actual plant performance; and
– simulated performance, available for comparison with actual performance.

Note: Parameters are determined at actual process conditions. If the optimization were to force the process into a different operational point, it would require an additional optimization cycle before updated parameters could be incorporated into the optimization.

If gross errors are detected they might be eliminated from the measured set, and the DR&PE might be repeated as described under DR in the previous paragraph.

At this point we exclude the model validation, which is discussed during the methodology description (see Section on Validation 9.6.12). In the optimization cycle it is assumed, that the model has been validated.

Simultaneous data reconciliation and parameter estimation will provide the best fit between actual and simulated performances, as the reconciliation emphasizes an extended set of measured data covering the rigorous model. The precondition is that enough redundancy is available in the plant measurement not limited to DR but also for PE.

The model The entire empirical or fundamental model form the bases for the estimation. The factors to be addressed during model building are:

- Selection of commercial flowsheeter equation-based, provided with model library, physical property data bank, optimization routines and economic section.
- Overall process model, empirical versus fundamental.
- Reactor modeling – are there kinetics available at sufficient detail?
- Projected accuracy of the model. The level of detail of the model, partly determined at the feasibility stage (see Section 9.6.1) but also during model building, to comply with model accuracy requirements.

- The application of suboptimizations is to be decided during the control strategy design as it has an impact on the model.
- Constraints to be modeled – constraints are either handled in constraint controllers often based on direct plant measurements, or they are modeled. This differentiation must be made during the design of the control structure.

Process units have, for most of the time, more than one constraint. Although it should be noted that in general there are only a few process units that are limiting for the operation, these often have more than one active constraint. The number of potential constraints of a simple distillation tower is listed in Table 9.1. The potential constraints for a furnace are illustrated in Figure 9.10. It is clear from these lists that different constraints might be restrictive under variable conditions (White, 1999). For the example of the distillation, the actual operational constraint list may seem much shorter. Often, the pressure in the column is a limiting factor as a result of limited capacity of the reboiler/condenser next to flooding or weeping limitations in the column. A representation of the constraints of a column itself is shown in Figure 9.11. However, be aware that during optimization the column might run into different constraints at different operational conditions. Flooding in the bottom, feed or top section based on gas and liquid loads may be practical limits, but weeping may also be a constraint:

- Feed slate, product slate ranges, feed and product and utility specifications.
- DOFs for the optimization.
- Parameters to be estimated or calculated during operation.
- Price range projection.
- Robustness over the entire operational range.

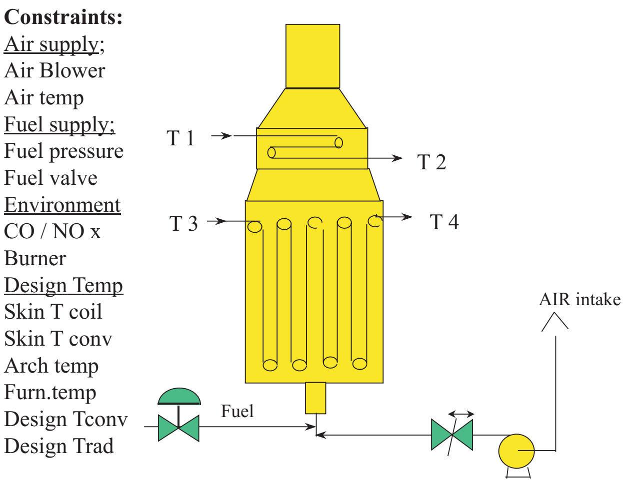

Fig. 9.10. Furnace constraints.

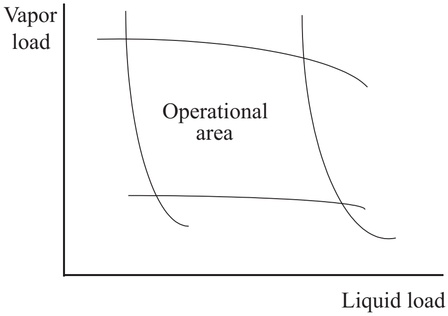

Fig. 9.11. Constraints of a distillation column.

Table 9.1. Constraints of simple distillation column.

Process	Bottom temperature (decomposition)
	Top temperature (solidification)
Column	Design temperature
	Design pressure
Internals	Flooding and weeping of top section and bottom section
	Gas loading (high and low)
	Liquid loading (high and low)
	Overload at feed section (high and low)
	Pressure drop
Reboiler	Fouling
	Heat source temperature and pressure
	Design temperature and pressure. Shell and Tube
Condenser	Fouling
	Cooling medium temperature and pressure
	Design temperature and pressure inside and outside
Reflux drum	Design temperature and pressure
Instrument measurements	Range
Instrument actuators	Capacity/range
Lines	Design temperature and pressure
	Pressure drop
Pumps	Design temperature and pressure
	Capacity and head

The final result of the model should be accurate and robust over the entire operational range. The model must be tested in combination with the optimizer, and demonstrate its robustness from different starting points.

At the feasibility stage (Section 9.6.1), the factors that play an important role in the overall economic process performance are identified by sensitivity analysis. Also, the constraints that have an impact on the overall operation are identified at different operational conditions. During model building these factors must be properly reflected in the model. The model might be very detailed for one unit, with a detailed description of all the constraints to be encountered at different conditions. On the other hand, it may be very elementary for another unit because it only has marginal impact on the economics and does not encounter any constraint. In this last case, one might think about a distillation column or stripping column that could be formulated in split factors with an energy term connected. The validation of the model is discussed in Section 9.6.12.

Parameter estimation Typical parameters to be determined include: compressor and column efficiencies; fouling factors or overall transfer coefficients of exchangers; and catalyst aging factors. These parameters are often only calculated as there is not enough redundancy built into the flowsheet for them to be estimated. The technique for the determination of the parameters is essentially the same as applied for data reconciliation, the Lagrange multiplier method generally being applied (see data reconciliation).

During the DR /PE the gross errors of a selected set of measurements are determined by specifying operational limits. One might decide to validate all measurements of the plant with this methodology. It should be realized however, that it would mean writing very detailed models. In addition, one would also need to be able to describe the product streams and its physical properties in detail. For example, the composition of a tar stream which might change at different feed or reactor conditions is often not known, but it will have an effect on the vapor pressure and as such at the bottom temperature or pressure of a tar splitter. Similar comments can be made about the impact of inertia, if the quantity of inertia is not accurately known, then the calculated dew point of a stream will not be reliable.

Decider 3 The decisions to be made at this point are:

- Is decider 1 true?
- Is decider 2 true?
- Are the estimated parameters available and within pre-defined range?
- Are the gross errors removed from the selected measurement set?
- Are the DOFs for the optimization still applicable (are the control loops for the implementation of the set-points of the optimizer still closed)?

9.5.2.4 Optimization

Updated model Three activities can be recognized:

1. The optimization step starts with updated model parameters.
2. The DOFs for the optimization need to be available for implementation..
3. The constraint are set/updated as far as these are not calculated within the model.

The constraints set are, or are coming from:

- operation such as the capacity of the process plant or product specification or receipt; these are communicated through the basic control system.
- from the control system, in case of operational constraints as experienced by the constraint controllers; this might be the maximum capacity of the feed or the maximum load of a refrigeration system.
- hard constraints already fixed in the program as design pressures, temperatures, product specifications.

Optimization Based on a robust model, the optimization is just run time, which limits the cycle time. The optimization always takes much more time than the previous steps if we exclude the time that the process takes to comply with the steady-state criteria for plant stability.

Decider 4 The decisions to be made before the new optimized set-points are released for implementation to the control system are:

- Is decider 1 true?
- Is decider 2 true?
- Is decider 3 true?
- Did the optimization converge?
- Are the calculated optimal set-points within the defined feasible range?
- Are the DOFs selected for implementation still available for implementation?
- Is the difference in projected performance versus last implementation optimization meeting a certain criteria? The calculated simulated profit might be within the noise range of the operation. The implementation of new set-points introduces a disturbance into the process, which always has some disadvantage. Therefore, a criterion might be defined based on projected saving versus the last implementation.

9.5.2.5 **Implementation module**

This downloads set-points that are made available from a latest optimization results. In this module are defined the ramp-up rates and the schedule of implementation at BC and MBC levels. In particular, the scheduling requires careful design as this might lead to hazardous or unstable areas.

9.5.2.6 **Overall sequence and operator interface**

The overall sequence is operated by an executive, that operates according to a schedule. The cycle as discussed above has the steady-state detection module always operable as long as the process plant is in the run step. The reconciliation step is also always operable, even if decider 1 is not true, but the process need to be in the run step. This means that the performance meter that is coupled to the reconciled mass balance operates, even if the plant is not steady enough from an optimization perspective. The mass balance reconciliation will have a correction for any variation of the hold-up and integrates over time. The parameter step is operable if decider 1 and decider 2 are true. The optimization step is operable if deciders 1, 2, and 3 are true.

The status of the different steps must be presented at the operator interface that requires the following information:

- A step flow diagram with indication of the activated steps.
- The last and recent released information from each step.
- Cumulative information of each step.
- An overview of the recent downloaded setpoints from the optimization in relation to the actual set-points and its measurement.
- An overview of the hierarchy of the control regarding the set-point downloading. The signal transmission from the model-based controller to the basic control layer and from the optimization layer to the model-based layer and the basic control layer. The overview needs to include the position of the control loops (closed or open).

Summary

Closed loop optimization is not a trivial effort, they are differentiated in several methods: self-optimizing control or sub-optimization, empirical optimization, and fundamental model based control. These methods are summarized as:

- Self-optimizing control, a unit optimization technique applied as a suboptimization is discussed with, as an example, a divided wall column. This is a promising, but quite new technique.
- Self-optimizing control is simple feedback system where the controlled variable has been selected based on steady-state analysis to obtain a system where the optimal value is:
– only weakly dependent on disturbances;
– sensitive to changes in independent variables; and
– easy to control accurately.
- Empirical optimization for processes with a few units and limited DOFs is presented for process where fundamental models are not available. The development of empirical models based on an experimental design applied to the existing process can only be successful if the process is adequately stable. Implementation might be off-line, but with quality loops closed. This technique has not found wide application although some parts of a fundamental model as applied for optimization may en-capsule an empirical model.
- Fundamental model-based optimization is the most widely used approach, as it brings process understanding that definitely leads to process improvements next to an optimized operation. Crucial to the development of the optimization models are: the reactor and unit operation models all written for an equation-based simulator, an accurate description of the constraints, its accuracy and robustness.

- The optimization cycle applied for the implementation of OO is discussed for the individual modules: data analysis, data reconciliation, simultaneous data reconciliation and parameter estimation, optimization and implementation of set-points. Each module is provided with an input block and a decision block after execution of its task.
- Data analysis primary tasks are described as: removal of corrupt measured data; steady-state detection based on defined criteria; and decision on progress to the next sequential module.
- Date reconciliation is based on the minimization of the deviation of the square of the differences between the reconciled values of measurements and the measured values. The model is based on the reconciliation of mass and heat balances. The calculated values are used for the performance measurement as described before, and to define the feed rates and composition of the process. The minimization can be done using the Lagrange multipliers method. During reconciliation, measurement errors can be both detected and eliminated.
- Simultaneous data reconciliation and parameter estimation is done on the entire process model to determine the value of those variables (parameters) that are subject to change over time or capacity. For this step an accurate validated model is essential, including constraint descriptions. The parameter estimation will be done in concert with data reconciliation of the full model, despite the determination of the feed rates and composition in the previous step. The result of this step are: detection and elimination of measurements with gross errors, estimated parameters (some of these parameters may just be calculated due to a lack of redundant measurements); simulated performance in comparison to the measured performance.
- Optimization of the updated model (adjusted parameters) must be done for DOFs which are accessible. Verification of the results and submittal for implementation to the implementation module must pass the final decision block.
- Implementation of set-points that are made available by the optimization is done through the implementation module. The module has the possibility to define the ramp-up rate of the individual set-point and the schedule for implementation
- Overall sequence and operator interface. An executive controls all the individual steps of the implementation, and requires a carefully designed interface up to operation that in one picture has a complete overview of the system status and its actions.

9.6
Project Methodology for Operation Optimization

The methodology for the implementation of an OO project is described. The overall step-wise methodology is presented in a flow diagram (Table 9.2), which emphases the successive steps to be taken for an optimization project. The details of each step are described in the subsections, and the methodology is described for the implementation of a CLO of a continuous process. Before a project is even started, a feasibility study must be prepared to define the scope, costs, savings, and the economics of a potential project. The project is concluded with an appropriate evaluation and an adequate maintenance structure. This section will be concluded with a short note about the implementation of off-line optimizations as well as dynamic optimizations.

Table 9.2. Project methodology, flow diagram for OO projects.

<table>
<tr><td colspan="2">(0) Feasibility study</td></tr>
<tr><td colspan="2">(1) Scope definition</td></tr>
<tr><td colspan="2">(2) Develop and install performance measurement and start tracking process performance</td></tr>
<tr><td colspan="2">(3) Develop control structure and CVs, MVs, DOFs</td></tr>
<tr><td colspan="2">(4) Build executive and implement data analysis for steady-state detection and performance meter</td></tr>
<tr><td colspan="2">Parallel activities</td></tr>
<tr><td colspan="2">Develop control develop model</td></tr>
<tr><td>(5C) Inventory of control improvements</td><td>(5M) Develop and validate reactor model</td></tr>
<tr><td>(6C) Design and install additional Instrumentation</td><td>(6M) Develop process model with reactor model including optimizer</td></tr>
<tr><td>(7C) Design and implement improved basic control and test plant stability and disturbance rejection</td><td>(7M) Test process model for robustness on process conditions and prices</td></tr>
<tr><td>(8C) Design and implement model-based constraint control test plant stability and disturbance rejection</td><td></td></tr>
<tr><td colspan="2">(9) Implement data analysis on selected data</td></tr>
<tr><td colspan="2">(10) Implement data reconciliation</td></tr>
<tr><td colspan="2">(11) Implement simultaneous data reconciliation and parameter estimation</td></tr>
<tr><td colspan="2">(12) Validate model</td></tr>
<tr><td colspan="2">(13) Implement closed loop optimization</td></tr>
<tr><td colspan="2">(14) Evaluate project and build up maintenance structure</td></tr>
</table>

9.6.1
Feasibility Study: Step 0

The elements of a feasibility study are discussed below, after provision of an overview of the elements to be addressed. The elements of a feasibility study include:

1. Objective of the study
2. Modeling background
3. DOFs for optimization and model-based control
4. Sensitivity of DOFs on process performance
5. Constraints identification
6. Parameters
7. Control performance
8. Performance measurement
9. Projected cost and time planning and manpower resources
10. Project savings and evaluation

9.6.1.1 Objective of the study

During the feasibility study, the different options for optimization should be explored and result in an estimated cost versus benefits analysis. The different options to be studied depend to a large extent on the type of process:

– For batch processes, scheduling and constraints control on the feeds must be considered to obtain shorter batch times.
– Continuous processes with consistent feed sources and pure products, efficiency improvement and capacity increase are target objectives.
– Continuous processes with different feed stock options, an improvement of the efficiency of operation at the different feed stocks is quite achievable. An OO project might include as a spin-off a feed stock evaluation tool which can generate considerable savings.
– Continuous processes with many transient operations for different product grades: scheduling, increasing capacity and reducing off-grade are subject to evaluation (this is particularly applicable to polymer processes).

The basic factor behind an OO project is the economic benefit achievable by ongoing adapting the process conditions at changing circumstances.

Variability An overview must be made of the variation in circumstances, and the frequency of occurrence which have an impact on the economic performance. This should provide input for the answer to the question of off-line versus on-line optimization. Variations might include feedstock and product variations, product distribution, price sets but also environmental effects. The benefits are to be found in more efficient operation including capacity increase. The capacity of a facility is only important if the business has a market for an increased production. On the other hand, an optimization can provide a cheaper capacity increment.

It should be realized that the implementation of an OO project takes between 18 months to 2 years. An approaching improvement project will have an impact on an OO project, and therefore should be considered during implementation.

The feasibility study should conclude with a list of potential project options to be explored in more detail. The next steps are explained for a static/dynamic OO project, and they all serve as back-up for the cost–benefit analysis. (Scheduling projects would follow another track, but this is not discussed here.) Most of the following activities will be worked out in more detail during the development of the OO project.

9.6.1.2 **Modeling background**

It is important to have the modeling background defined. The process modeling background is important, as most companies have modeling experience and simulations available of the process under study, with some preferred modeling software. This has an impact on the modeling effort to be performed, and also on the eventual software license cost.

Reactor modeling is a must to enable accurate OO models for processes with a reactor. The type of reactor models depends on the available knowledge – it may be empirical, a conversion model, or a fundamental model. It is the required accuracy (which is a function of the overall contribution of the reactor system to the process operational cost) that dominates the type of reactor model. A reactor that sets the product distribution of the process is most likely a prime candidate for a rigorous fundamental model. A reactor that operates at close to 100% conversion (e.g., hydrogenation of a di-olefin in the presence of olefins) can often be optimized locally by a self-optimizing controller. In such a case, a conversion model implemented in the overall process model might be sufficient. For commercially available processes, reactor models might also be available commercially. Often these are closed versions, in which case it is better to negotiate excess to the derivatives functions in order to enable optimization.

Although the cost of a reactor model can be high, is often a prerequisite for an OO project. It should be noted that the development and validation of a model requires stable process conditions and accurate measuring techniques that are normally not available in a process plant. This could be an argument to include these requirements in a OO project.

9.6.1.3 **DOFs for optimization and model-based control**

The DOFs for the plant-wide optimization are in general the specification of internal streams and the set-points for reactor conditions. These set-points will be downloaded from the OO executive to the MBC system or the basic control system, depending on who is controlling what. Sub optimizations such as self-optimizing control have to be predetermined at this step in relation to plant-wide optimization. A preliminary split must be made for the DOFs applied at the MBC or OO layer. Constraints are preferably approached by MBC, as they often take advantage of direct process measurements with avoidance of calculations. For example, if a condenser is subject to fouling, optimization does need to estimate a fouling factor and calculate the maximum exchanger duty in relation to the cooling medium, which might be subject to the outside temperature. The MBC might use the pressure in the system as input to a constrained condition caused by heat exchangers. The quality of product streams might be a constraint, and as such input for the MBC; however, the value of the constrained quality might also be subject to optimization. The exercise results in a preliminary balance between MBC and OO activities. During the project development the borders need to be further defined.

9.6.1.4 **Sensitivities of DOFs on process performance**

The sensitivities of the DOFs on process performance set the basics for the economics of a OO project. The sensitivities are determined quantitatively by perturbations of the DOFs selected for the optimization of the overall process or process model. The sensitivities need to be explored over a larger range of the operation, as currently practiced. Most OO projects are forced against constraints, which are likely to be outside the existing operational range.

9.6.1.5 **Constraints identification**

As mentioned earlier, OO will force the process against constraints, and these will be different under different economical conditions. The constraints are partly determined during test runs, and partly by calculations, as the processes will not be available for all extremes of conditions. The most important constraints are capacity constraints, particularly at different feed-stocks and product distributions. Be aware that the maximum operational conditions as experienced by operation personnel are approximately 5–10% removed from the real constraints. Operations not equipped with constraint controllers will operate with conform zones that are the challenges for OO. Capacity constraints are often subject to meteorological conditions; for example, the daily temperature cycle might be a cheap capacity increment (see Figure 9.3).

9.6.1.6 **Parameters**

The parameters that must be estimated or back-calculated during the simulation/optimization are those which are subject to change during extended operation, and have a noticeable impact on the economic performance. The obvious parameters include: compressor efficiencies of larger machines; column efficiencies; reactor aging; and fouling factors of exchangers as far as they have an impact on process efficiency or constraints imbedded in the optimization.

9.6.1.7 **Control performance**

For the implementation of the OO project, a robust controlled operation is a requirement. During this step the quality of the control should be monitored and the amount of upgrading of the basic control layer be determined. An estimate of the number of MB controllers needs to be prepared based on suboptimizations, constraints and decoupling of interactions to be addressed. The analysis will also identify additional instrumentation to be installed for parameter estimation and performance meters.

9.6.1.8 Performance measurement

The performance measurement is discussed in Section 9.4. In this step, it is important to determine the development costs and the additional instrumentation required to perform this functionality.

9.6.1.9 Projected cost and time planning and manpower resources

The determination of all the costs involved in the implementation of an OO project are a requirement, and to assess completeness, the following list is prepared:

- Modeling software costs to be included; licensees for process simulator, reactor models, optimization executive, model development.
- Control software costs to be included; licensees, redesign basic controllers and its programming, model-based controller development and installation.
- Hardware costs involve instrumentation, computer platform for MBC, and optimization.
- Implementation costs and validation.
- Maintenance costs, mainly updating of models.

Time planning is an important factor, as the total execution time might be more than 18 months. Also, the involvement of company-related manpower should not be underestimated, in terms of availability and cost.

9.6.1.10 Project savings and evaluation

Savings are determined in perspective of the maximum achievable savings for the objected optimization. The approach for the different OO projects will differ slightly.

Scheduling projects will determine the savings related to the maximum achievable operational schemes (no waiting times between batches), but including flushing steps if required.

Transient operational savings will be estimated by comparing the actual and minimal transient times that determine the off-grade production, as well as the capacity gain during transients. In general, the minimization of the transient operation is constrained in the process. Minimization might be restricted, in case of co-monomer grades, by the feed capacity of one of the co-monomer systems to obtain the new required concentration in the reactor system.

Continuous operational savings can be split into capacity maximization and conversion cost reduction. Capacity maximization must be estimated from the constraint analysis with different feedstocks and product states, in addition to the potential capacity gain by taking advantage of varying meteorological conditions (e.g., temperature day and night cycle). Capacity gains on the order of 5% are easily achievable, particularly in the case of multiple (three to five) constraints, while alternative feedstock options (two to three) may increase this by up to 10%.

Conversion cost savings are estimated as a percentage of the conversion cost. White (1999) used the following approach, based on experience:

- Savings of a factor 0.05 up and to 0.1 times the raw material cost gap between actual and theoretical feedstock cost.
- The factor 0.05 was used for systems with 1–5 independent variables for optimization.
- The factor 0.1 was used for systems with a large (25) number of independent variables.

Reduction in operating expenses (including utility costs) will be factored by 0.05 to 0.1 of the total operating expenses. Like the factor for feedstock saving, this factor will similarly depend on the number of independent variables for OO.

A more fundamental approach was developed by Hennin and Perkins (1994) and by Loeblein (1997) and Loeblein and Perkins (1996). This approach has been validated by Vafiadis (1998) and Loeblein and Perkins (1999). The method is based on the availability of an optimization model applied for off-line OO. The ultimate optimization results can be determined if the constraints and the parameters are determined precisely over its operational range. The back-off for actual CLO from the ultimate optimization can be determined based on two factors; the uncertainty of the optimization, and the control performance. In other words, the average deviation from the ultimate optimum for an on-line optimization depends on; the covariance of the statistical uncertainty in the parameters and the measurement errors, and the regulatory control performance. The theoretical approach has been verified by the application of Monte Carlo simulations.

This method assumes that an off-line optimization model is available and that the constraints and parameters are known, next to the measurement accuracies. This information is not available at the start of a OO. project. For the determination of the savings of a CLO in respect of an off-line optimization, it will have its benefits.

The economic evaluation of an OO project must be based on a cost–benefit analysis. The technical evaluation regarding manpower, software, hardware and maintenance consequences should be clearly considered as these might have technical and organizational impacts. Site or company standards might be affected by decisions regarding software and hardware.

9.6.2 Scope Definition: Step 1

The definition of the scope should include the following elements based on the feasibility study results:

- Type of project (static/dynamic; optimization/scheduling).
- Type of optimization (off-line/closed loop).
- Type of software for flowsheeter/reactor modeling/executive.
- Preliminary selected DOFs for optimization
- Boundaries of the project.
- Cost, timing and manpower allocation.
- Projected savings.

For the technical details, reference is made to the feasibility study, although many technical details will need to be obtained during the modeling and the control design.

9.6.3
Develop and Install Performance Measurement and Start Tracking Process Performance: Step 2

The performance measurement is one of the first attributes to be installed in the process plant. The design of the performance meter is described in Section 9.4. One of the most important functions is to track the performance of the process before optimization is installed. This will be the baseline for the evaluation of the project. During these observations, we most likely measure the performance of the process at fixed price sets. The accuracy of the process model to be achieved is not yet known, but the savings are already estimated and these should be measured at least at an accuracy of 10%. This sets the accuracy of the performance meter.

9.6.4
Develop Control Structure with CVs, MVs, and DOFs: Step 3

The overall control structure with a split between basic control (BC), MBC and optimizer manipulating set-points is determining the control activities. Examples of control configuration for a simple distillation and a reactor system are given in Figures 9.12 and 9.13 and are represented in Tables 9.3 and 9.4.

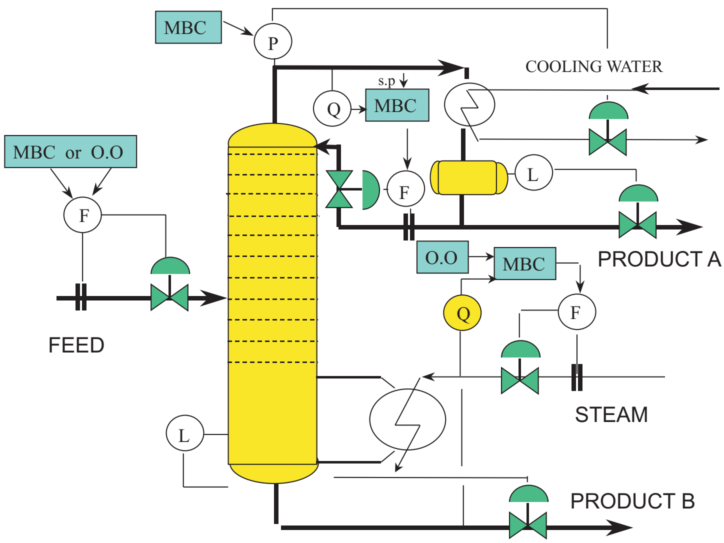

Fig. 9.12. Control hierarchy round a distillation column.

Table 9.3. Example of a typical control configuration for simple distillation (see also Figure 9.12).

Basic control layer	
CVs	MVs
Feed flow	Feed valve position
L top	Distillate valve position
L bot	Bottom valve position
Reflux flow	Reflux valve position
Steam flow	Steam valve position
Pressure	Cooling water valve position
MBC layer	
CVs	MVs
Capacity maximization	Feed flow set-point
Floating pressure	Pressure set-point
Q bot	Steam flow set-point
Q top*	Reflux flow set-point
OO layer	
CVs	MVs
Profit	Q bot set-point
	Feed flow set-point optional

* Quality of top stream is seen as a constraint not subject to optimization

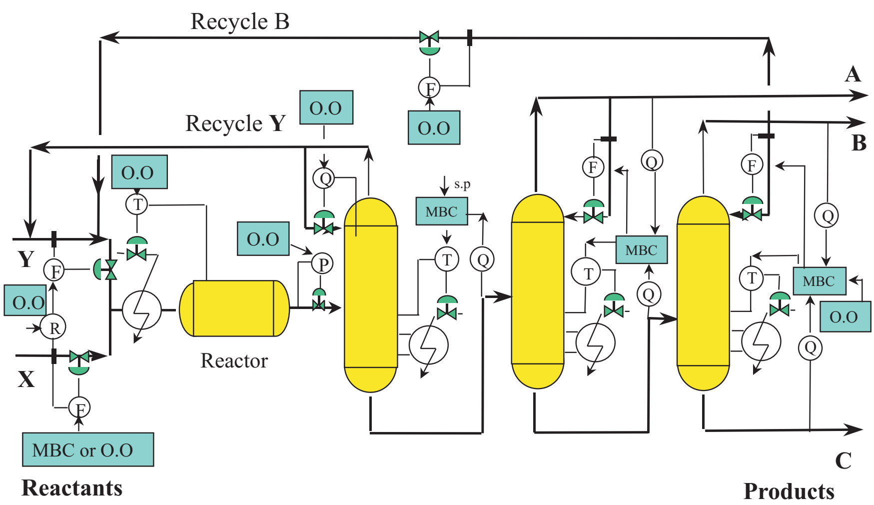

Fig. 9.13. Control hierarchy of reactor and finishing section (level loops at overhead and bottoms and pressure control are not shown).

Table 9.4. Example of a control configuration of a reactor and distillation finishing section (see also Figure 9.13).

Basic control layer	
CVs	MVs
Reaction section	
P reactor	Pressure valve position
T reactor	Steam flow valve position
Flow reactant X	Reactant X valve position
Ratio Flow X, Y	Reactant Y flow set-point
Reactant flow Y	Reactant valve position
Recycle flow B	Recycle valve position
Distillation section	
Level top sections	Distillate flows valve position (not shown)
Level bottoms	Bottom flows valve position (not shown)
Temperature bottom sections	Steam valve positions
Reflux flows	Reflux valve positions
P top	Cooling water valve position
Q top first column	Reflux valve position
MBC layer	
CVs	MVs
Capacity	Feed flow set-point reactant X
Q bottoms	Temperature bottom set-points
Q top*	Reflux flow set-points
OO layer	
CVs	MVs
Profit	Ratio set-point reactants X and Y
	Temperature set-point reactor
	Pressure set-point reactor
	Recycle flow B set-point
	Q bottom product C, set-point
	Feed flow set-point reactant X, optional
	Q top set-point, first tower

* Qualities product A and B are considered as constraints not available for optimization

In the example of simple distillation, the qualities for top and bottom were supposed to be manipulated by respectively reflux and vapor, while the levels were controlled by distillate and bottom flows. This is just an assumption for this example; in reality, the basic control configuration needs to be designed and the optimal pairing for the control selected (see **Chapter 8**.) The top quality is seen as a fixed product specification, a hard constraint, while the bottom specification is seen as a recycle with an adjustable specification depending on plant economics. The pressure is controlled by the cooling water.

The MBC is manipulating the set-point of the steam reboiler and the reflux flow set-point for de-coupling of the interaction to achieve dual composition control as self-optimizing controller.

The objective of floating pressure control might be implemented in the MBC system, but may also be incorporated in the basic control layer (Shinskey, 1988).

The set-point of the feed flow might be set by three different sources:

1. Manual operator set-point for capacity.
2. MBC constrained capacity (maximization)-
3. OO constrained operation.

The set-point of the feed flow is a target of the MBC in case of feed maximization, as far as the set-point is available and the constraint(s) have been defined. For instance, floating capacity control to maximize the production under the day and night temperature cycle, applicable if environmental (in)directly cooled exchangers are the constraints. Also, the feed might be constrained by flooding to be identified by a column pressure difference measurement. The representation of a capacity maximization with floating pressure according to standard control notation is shown in Figure 9.14. The feed flow set-point is a target which might be derived from a plant-wide optimization layer. OO selects the optimal set-point for the bottom quality.

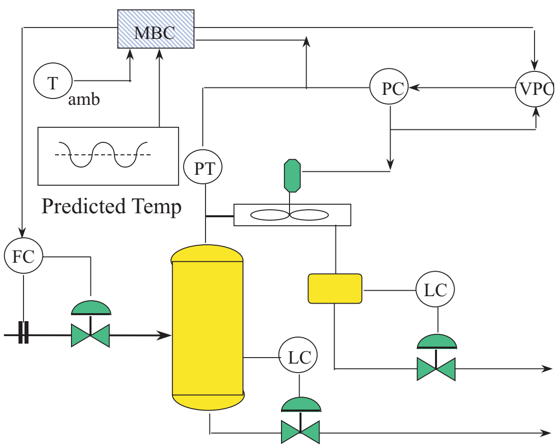

Fig. 9.14. Floating pressure control with capacity maximization based on predicted ambient air conditions.

In the example of the total plant control (Figure 9.13 and Table 9.4), a reactor and three finishing towers are shown. The pressure control planned with the overhead condensers is not shown on the flowsheet; neither are the level controllers on the overhead drums and the bottoms. The products A and B have a hard quality specification.

The following set-points are controlled by MBC: The quality controllers of top and bottom streams of the distillation towers; and feed maximization for the reactant X.

OO manipulates the set-points for the feed (optional) and the ratio of the reactant Y versus X, the recycle flow of product B, the reactor temperature and pressure, the quality of recycle Y, the quality of product C.

The choices of who is controlling what has an impact on the modeling activities for MBC, as well as for OO, particularly in relation to the description of the constraints. The objectives for BC are stable operation with hard specification quality loops closed, and the soft quality loops open in case of interaction. This is based on the control design philosophy of Luyben et al. (1998), who phrased it as:

It is always the best to utilize the simplest control system that will achieve the desired objective.

To differentiate BC from MBC, the author introduced the following concept:

Basic control design has conceptual to be simple and easily operable in case of failure of a higher control layer.

The above statement includes a preference for the self-optimizing control approach at the basic control level, as is advocated by Skogestad.

The objectives for MBC in steady-state optimization are: self-optimization of units, decoupling of interaction, constraint control like capacity maximization and model predictive controllers to achieve better control particular for transient operations like batch reactors.

The objectives for OO are: optimize operation by downloading optimal set-points or transients operations trajectories from process-wide optimization simulations.

It is the executive who, depending on the situation, sets the decision as to which controller is active for implementation. The communication lines are illustrated for the different layers in Figure 9.15, which shows that OO may send set-points to MBC as well as to the BC layer, and also receive information from both systems. In case of an outage of a specific MBC function (as in the example of the bottom quality controller), the OO may still function. It can perform its function with a DOF less or, it can determine optimal bottom quality and select the corresponding set-point of the steam reboiler flow with an additional margin, to avoid off-spec situations as a result of dynamics. All the above situations need to be considered and implemented through the executive.

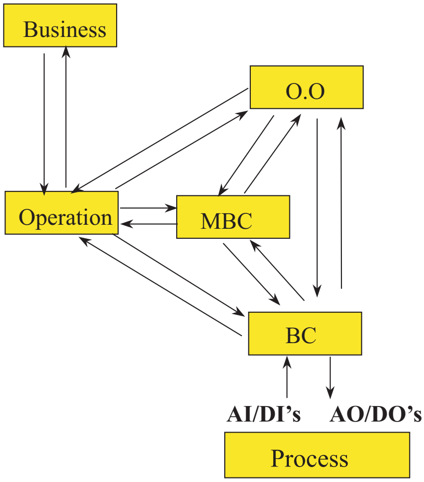

Fig. 9.15. Communication plan between BC, MBC, OO, Operation and Business.

The above illustrates the need to define clearly the premises for BC, MBC and OO, and who is doing what. The premises for the control design are the following:

- A lower level of control should be able to function independently of an outage of a higher level control.
- Basic control should be designed simple and robust with a high disturbance rejection capability and require a minimum of operator attention during outage of a higher control level (MBC and OO).
- The hierarchy of the control configuration should be clearly defined and, in an actualized format, presented to operation.
- Operational input should be implemented through one workstation to approach BC/MBC/OO.
- Higher control layers always send their outputs to the basic control layer, and will not directly activate a AO or DO.

9.6.5 Build Executive and Implement Data Analysis, for Steady-State Detection and Performance Meter: Step 4

The executive operates the optimization cycle as discussed in Section 9.5.2. The software framework for this functionality is available commercially. During development of the OO, the executive will be implemented and the individual steps tested and evaluated step-wise.

The implementation will start with the performance meter, at which point the data analysis based on improved control design is not yet available. The performance meter will initially be based on the average data over a longer time period to smooth the dynamic effects.

The next step will be the selection and implementation of the Steady-state Representing Values (SRVs) (Krist et al., 1994). The selection of SRVs is based on process insight, and should be representative if the overall process is to be considered at steady state. Some guidelines for selection include:

- Major process flows
- Pressure is a good indication of stability; preferred pressures are inlet and outlet pressure of units, top pressure of distillation columns and pressure difference representing the process condition of the unit operation (not the head of a pump or liquid levels).
- Suction pressure and revolutions in time of compressors (including refrigeration machines). In the case of a floating suction pressure, the discharge pressure might be selected.
- Temperature measurements representing the overall unit performance, like inlet and outlet temperature of an adiabatic reactor and a peak temperature (not necessarily fixed to a location), the temperature of a CSTR reactor. Do not take a temperature measurement which might be impacted by inertia or heavy streams of which the composition might change (and thus its temperature). Temperatures that are influenced by pressure should have a pressure compensation before use as SRVs. Specifically, vapor liquid equilibrium units which are subject to floating pressure operation.
- Quality measurements on essential process streams having an impact on product distribution and quality.
- Units with a very large response time; for example, liquid–liquid extraction columns, distillation columns with large numbers of trays and high reflux ratios should be judged on the stability of product quality and less on recycle quality. This to avoid too much time being lost before the next optimization cycle can be implemented.
- Levels in accumulators are purposely varied, and therefore should not be selected as SRVs (as for pump pressures).

Implementation of the data analysis and development of the filtering and stability criteria can only take place after the control design improvements have been implemented. Control design as required for steps 5C, 6C, 7C is discussed in **Chapter 8**, while the design of model based controllers step 8C is considered outside the scope of this work.

9.6.6 Development and Validation of Reactor Model(s): Step 5M

The development of the reactor model is, for most process optimizations, one of the crucial steps. The reactor in most processes has a major impact on the overall optimization. Several different ways exist to deal with reactor models, including:

- The model has been developed internally.
- The model is described in the literature.
- The model is available commercially.
- The model needs to be developed.

The models might be available in empirical or fundamental forma. The crucial questions is whether it has the required accuracy to contribute to the optimization. It was argued previously that the contribution of optimization to operational cost savings is in the order of a few percent. Therefore, the reactor model needs to meet (in most cases) a high accuracy. The development of a fundamental model is, in general, a research activity which is not discussed at this point in time. However, the development of an empirical model and the validation of reactor models will detailed in the following text.

The development of an empirical steady-state reactor model might be based on input/output analysis of the process. The technique to develop these emphasizes the following elements:

- Development of an experimental design program, including all operational degrees of freedom.
- Accurate measurements of all relevant process conditions and feed and product compositions.
- Process stability during testing.
- Selection of the proper parameters to update the model for ageing over the life cycle of the reactor (catalyst).
- Modeling is preferably done as a regression model where the equations still have a sort of physical representation, including parameters and which obey mass and energy conservation laws.

As was proposed at the feasibility step, the specifics of the reactor and the contribution to the economics, set the effort and the accuracy requirements. The development of such a model depends heavily on process stability, the operational experimental range, and the measurement accuracy. Particular measurements and analytical techniques often need to be installed and developed before the model development can effectively start.

The validation of a reactor model (fundamental as well as empirical) is seen as a separate effort from the overall process model validation. This is particularly so as specific measuring and analytical techniques are involved which include measurement of impurities and product properties (as in polymers) that can have a major impact on the process. Fundamental models developed based on laboratory data also need to be validated in the plant to confirm their validity at plant conditions.

The technique is based on minimization of the square of the deviation between measurements and prediction. The degrees of freedom for the developer to cope with mismatch are limited, and include:

– The determination of model variables as; activation energy, frequency factors or the reaction scheme for fundamental models, updating flow characteristics as dispersion coefficients or mass/heat transfer coefficients.
– The selection of parameters for updating over (aging) time.
– Extension of the operational range of the validation; this is frequently done at laboratory scale, but at plant scale the options are severely restricted.

9.6.7
Develop Process Model with Reactor Model, Including Optimizer: Step 6M

The process model in general is developed in an equation-based commercial simulator. These simulators are provided with library models, physical property data banks and equations, economic section and optimizers. To include the reactor models these also have to be written equation-based. Based on the results of the feasibility study, the detailed process flowsheet model needs to be developed and to cover the selected DOFs and constraints. The factors which play a major role in the level of detail are:

- Required optimization accuracy.
- Degrees of freedom as feed stocks, product slide.
- Constraints defined in the OO models versus the MBC.

It is advisable to make an overall process model (including the reactor model), but not up to a large detail, as unit operation can be described in a simplified way. The next step will be to replace the simplified unit models with more rigorous models, for those sections which have a major contribution to the operational cost. The units that will form a constraint are also candidate for a more detailed representation in the model, as far as the constraints are implemented in the optimization model.

During the development of the process model, we might extend the sensitivity analysis as performed during the feasibility stage regarding the impact of constraints and DOFs on the optimization results. This might result in additional constraints, DOFs and parameters.

The process model is built up unit by unit, and these unit models are verified against process data. Parameters such as tray efficiencies, mass transfer coefficients, furnace efficiencies, heat transfer coefficients are calculated and verified to match model versus process unit. Parameters can be differentiated according to the way they are handled:

- fixed at a constant value, determined during verification of the unit model;
- fixed, but capacity-dependent, as compressor efficiencies;
- updated during operation, particularly those that vary subject to fouling. Updating might be done by back-calculation or by estimation of the parameters. In the last case, the redundancy in measurements required for estimation must be available.

The unit models are combined into sections. The robustness of the section models must be tested before they are combined into the total plant model. The testing is done by variation of feed rates and compositions, but also different product specifications. Lack of robustness is often a signal for a modeling error. During testing of the section models, prices might also be connected to the individual streams to have the optimizer search for a quasi optimum (this is optional). Exploration of the model constraints under extreme process conditions is a worthwhile exercise that is not a trivial effort. The final step in the model building is the connection of the different sections and addition of the economic section and the optimizer. At this point it is a good time to replace some simplified models by more rigorous ones.

9.6.8 Test Process Model for Robustness on Process Conditions and Prices: Step 7M

The robustness of the optimization is crucial for final success. Failures to converge will result in no update of the values for the DOFs and as such would undermine the trust of operation and the success of the project. The overall model needs to be extensively tested for variations in feed rates, feed composition, product specification, prices and all other variables that might be subject to change. Bouncing against the constraints is another exercise that needs to be explored extensively, as reflected in the model. These exercises provide valuable information about modeling shortcomings (see also under the validation step).

9.6.9 Implement Data Analysis on Selected Data and Evaluate Steady-State Situations: Step 9

Implementation of the executive, with its different functions, is an effort which leads gradually to CLO. The successive steps are implementation of steady-state detection, followed by data reconciliation, parameter estimation, and model validation. All these steps are required to evaluate the quality of the control effort as developed under steps 5C–8C to achieve as stable operation and the quality of the modeling effort, steps 5M–7M.

After the selection of the SRVs (as discussed under step 4), the data must be analyzed. For each of the SRVs, analyses are performed on both raw and filtered data. The selection of criteria for the data filtering are the elimination of high-frequency process and instrument noise.

The selection of criteria for the average signal is impacted by the stability of the units and the overall process. The whole project is set up for steady-state optimization, so the plant should represent that state. The control loops as planned for BC and MBC levels need to be closed at this step based on appropriate design and tuning. Evaluation is carried out by setting stability criteria for decider-2 and tracking process stability over time.

9.6.10 Implement Data Reconciliation: Step 10

Data reconciliation is applied for:

- Performance meter (step 2)
- Estimation of input data for the simulation such as feed flow and composition, energy flows
- Gross error detection

All these functions need to be tested and the criteria set before moving to the next step.

9.6.11 Implement Simultaneous Data Reconciliation and Parameter Estimation (DR and PE): Step 11

DR and PE is performed to achieve a close fit between simulation and the actual operating process. The reconciliation and estimation is only possible in case of redundancy in measurement. Often, redundancy is insufficiently available, and in that case the parameters are calculated values based on process measurements. The technique of DR&PE is identical, and is described in Section 9.5.2. The parameters might be capacity-dependent. The procedure followed is that the parameter is determined at the current state of the process and updated every optimization cycle. This includes an off-set in the parameter if the capacity of the process has changed significantly, although at the next optimization cycle the parameters are updated. The selection of criteria for gross errors of measurements are based on the same criteria as for the data reconciliation module. Decider-3 also has criteria for outliers between simulated and actual measurements. The latter can only be selected after the model validation (step 12) has been performed.

9.6.12 Validate Model: Step 12

Model validation is an activity designed to minimize the difference between simulation and actual performance (J. Krist et al., 1994). The assumption for the validation is that the unit models were initially verified and the model has been demonstrated to be robust. The validation is performed in different steps:

- Gross modeling error detection.
- Smoothing of the model, by data reconciliation (DR) and parameters estimation (PE) on an extended set of measurements.
- Overall model validation, by comparison of simulated performance with measured performance.

The validation process contains similar elements for the different validation steps:

- Selection and calibration of plant measurements.
- Development of an experimental design program over the entire operational range.
- Interpretation of the results.

The different validation steps will partly run in parallel, but ultimately they are executed in sequential order.

9.6.12.1 **Gross modeling error detection**

This is a manual activity and, in principle, all deviations except for measurement errors are modeling errors. Measurement errors are detected by evaluation of its location (is it really located at place it is supposed to be?) and calibration (specifically for the validation). For validation, specific samples might be taken and analyzed on composition to confirm certain critical process streams. The ultimate effort is to minimize the square of the deviations between simulated and actual measurements. The focus in this step is on improvement of the process model after verification of the instruments.

The unit operation models include reactor models which have already been verified during the model building, and should be revalidated first. This is particularly so as the steady-state detection and data reconciliation and DR&PE modules are now operational. This makes it possible to achieve a better basis for comparison. The measured, simulated, and reconciled values of the individual units are collected for statistical validation over a number of weeks, with variable operational conditions. These collected data are mapped in linear steady-state models for flows, temperatures pressures and others, representing the simulated and the measured data, see Figure 9.16. Matching of these data shows the average slopes, intercepts, and spread. The results should be the identification of modeling deviations.

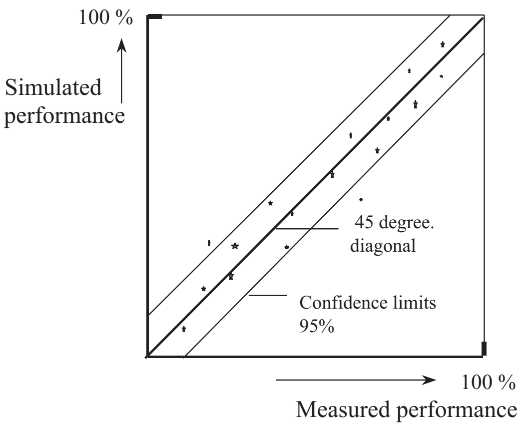

Fig. 9.16. Measured versus simulated performance, as variable operating margin, at a fixed price set.

Some (but not all) of the modeling errors include estimation of physical properties, clustering of components, parameters depending on load (e.g., heat/mass transfer coefficients), fixed parameters need to be determined over time, constraints ill-defined, inertia not foreseen, nonideal flow conditions, nonideal separations, etc.

After revalidation of the unit models the overall process model is to be validated. One of the major concerns at that point is that of the main process streams. Errors in overall streams often do not show up to that extent in the unit models. An example is a partial condenser splitting a major mixed hydrocarbon stream, which depends heavily on composition, temperature, physical properties and the efficiency of phase separation. A small error may send a different flow and different composition to another section.

9.6.12.2 **Smoothing of the model**

This step will be executed partly in parallel to the gross modeling error detection. At this stage, we will perform off-line simultaneous DR&PEs with an extended set of measurements and parameters, including those which were planned to be fixed in the validated model. Kinetic constants for reactor models might also be freed up for estimation, to obtain improved mapping between the simulation and the actual plant operation. With the collected data sets, iterations might be executed between model corrections (updates) and updated parameters to obtain the best fit.

9.6.12.3 **Overall model validation**

The overall validation is to be concluded with the performance meter (profit meter). The performance meter is based on mass balance reconciliation and the values of the different input and output streams. The results are expressed as a process performance in money per unit of time based on raw material, product and energy prices. It was concluded at an earlier stage that the profit meter needs no validation of the underlying model as it is based on the conservation laws. The noise of the profit meter is an important piece of information as it gives the deviation in the measurement due to measurement errors and process (un)stability (process noise). In case the spread is too large, this most likely will be caused by process stability, with an exception for profit meter design errors, (see Section 9.4).

There are several options to improve the spread of the performance meter due to process instability:

- Apply a larger integration time.
- Sharpen the stability criteria for decider-1.
- Improve the control.
- Include hold-up variations in the design.

The results of the mass balance reconciliation are also used to determine the flows and composition of the feed streams for the simulation. The overall simulated process performance can be calculated from the process streams at the same stream values (prices); this calculation should be part of the output of the optimization. The spread of the simulated performance is measured for the same price set as for the measured performance. The spread should be of the same order as the spread of the measurement.

The operational margin inherently provides a good overall image of the model when mapped against the measured function, since it represents values implicitly related through the equations of the model to be validated. The next activity is to collect a set of measured and simulated performance data over the operational range of the process for the same price set. Next, a plot is made between the simulated and measured performance over its operational range for a fixed price set (see Figure 9.16). A similar presentation was used for validation of individual measurements (see above). It is a requirement to evaluate the process over the entire operational range. The diagonal line represents the perfect fit between simulation and measurement. Lines are plotted in the same graph for the 95% confidence limits (or 1.96 times the standard deviation). A significant mismatch between the slope and intercept, together with a large spread, are indicators for the overall process invalidity.

Modeling mismatch During model validation it will become clear that there are – and there always will be – differences between the actual process and the theoretical model. Mismatch might be caused by errors in the model development, but also by nonideality in the process. We might regard these mismatches as being acceptable for the optimization, but they must be included in the decision criteria of decider-3. Some of the mismatches might be caused by the following reasons:

- Availability of inertia, which has an effect on the dew point of vapors.
- Composition of a heavy stream; often, heavies are determined in the feed stream or at the reactor outlet as a cluster of compounds. The composition of the stream might change, resulting in a deviation in vapor pressure.
- Accumulation of impurities (not included in the model) in process streams that might result in differences in temperature and pressure.
- Fixed parameters which depend on the capacity of the unit or fouling/aging; in that case, the parameter should be updated.
- Insufficiently described and validated unit models

The model mismatch does not necessarily have a notable impact on the overall optimization results, but it will have an effect on the difference between individual process measurements and simulation results. It is important to recognize these effects and to eliminate these measurements as SRVs and as part of decision criteria in decider-3. After a simultaneous data reconciliation/parameter effort for the total process model, the consistent outliers due to model mismatch need to be removed to optimize the fit. These deviations will have a negative effect on the updating of the simulation before optimization.

9.6.13 Implement CLO: Step 13

The updated rigorous model with adjusted parameters is used for the optimization with the selected optimization routines. The final result of the optimization must pass the criteria set in decider-4. Initially, deciders-1, -2 and -3 need to be true, and the optimization run needs to be converged. Some processes lift the process stability criteria, as set in decider-1 for data reconciliation and parameter estimation, for the implementation of the optimization results. The DOFs used for the optimization need still be available for set-point implementation; if not, then the optimization run must be restarted with the available DOFs. Another criterion is that the difference between simulated performance and optimized performance should be outside the standard deviation of the simulated results in order to avoid unnecessary process disturbances. The results of the optimization provide new set-point available for downloading to BC and MBC. These set-points are implemented through the set-point implementation module. The implementation of a set-point can be done gradually, by applying set-point rampers, or as a step change. The implementation of all set-points will follow a defined scheme

9.6.14 Evaluate Project and Build-up Maintenance Structure: Step 14

The evaluation of an OO project starts from the moment the project begins. During the feasibility stage, cost and the savings of the project are estimated. Cost can be tracked during the project; external costs can easily be determined, but internal costs requires book-keeping of internal hours. The savings are more difficult to determine, particular as most suppliers of this technology do not have a real interest in measuring process performance. This was one of the main reasons why the performance meter was introduced. Another reason was to develop a tool for validation of the optimization model. The savings are determined by measuring the process performance before the implementation of a project. The data of the mass balance reconciliation and the operating margin are collected ongoing, and can be used for the evaluation for different price sets at a later date, during and after the project.

The performance meter can also be used for the evaluation of other project aspects, such as hardware, and also the contribution of control projects such as the control part of the OO project. Savings can also be determined to some extent after the outage of an OO. The results are somewhat debatable, as operation also learns from the optimizer. However, with a performance meter in line a good indication of the savings can be achieved:

Maintenance The maintenance of an OO project is not trivial, and the benefits can only be continuously achieved by ongoing maintenance. This has several different aspects, including instrumentation, control, model updating and ongoing operation attention.

Ongoing operation attention looks simple, but it is not unusual that some apparently minor modification is not noticed (at least from the perspective of the OO). One might think about modifications in piping, equipment location, constraints, control configuration or tuning (less steady state) or feedstock selection. A solution might be to appoint the responsibility to a professional for most large process plants such as refineries, and indeed this is common practice.

Instrumentation maintenance must concentrate on signal analysis. If instruments are selected and installed according to the latest practices, calibration is no longer required and element reliability is very high and maintenance is less of an issue. Analyzers ask for a higher level of ongoing maintenance, although automatic checks and calibrations are now available and are a major step forward, although sampling and injection systems as applied for GCs are maintenance intensive.

Control demands ongoing attention to assure that control loops remain closed and stable. The principle that operation should not touch control actions is a precondition also for BC to maintain correct functioning. Any modification in the plant might ask for updating of the control design, and should be seen as part of the project.

Model updating is an effort like that of model-based control design, and requires a high-tech detailed process and modeling knowledge. The models require updating for any change in the plant even it is only a temporary one, as it always impacts on the OO.

In the long term, an efficient maintenance structure is crucial to ongoing benefit from OO.

9.6.15
Other Types of Optimization

These include off-line optimization, mixed integer optimization, and dynamic optimization.

- Off-line optimization is often the first step before the successive steps to quality and constraint control, and ultimately CLO are taken (see below for more details). The model needs to meet a reasonable level of accuracy, and also needs a validation effort. Therefore, a performance meter is a requirement, but the process must also be sufficiently stable to achieve a reasonable validation, and estimation of the parameter which will be fixed in this model. The model, however, will in general describe the constraints not accurately but only in a very rudimentary form. Off-line optimization is mostly done if the frequency of disturbances in the economic environment is low, but it might be complemented with self-optimizing control.
- Mixed integer optimization (MILP and MINLP). Scheduling of operations is generally done in MILP. Also, blending operation as practiced in refineries and executed under fully automated operation are also mostly done in MILP. These MILP scheduling and operations activities are beyond the scope of this work. MINLP are performed for utility supplies such as power and steam.

These systems are subject to frequent changes due to demand, but even more due to the supply of external power at different price sets, like during peak hours and with switch-off contracts. At the same time, several power units might be available, often at so-called “hot standby” conditions as back-up. These systems described in a MINLP environment are provided with an optimizer and will include options to influence plant capacities for demand. The optimizations often run off-line and have a continuous advisory function to operation. The optimization in general receives on-line updated information about units availability and conditions; if required, parameters might also be calculated/estimated. As the site vulnerability might be heavily affected by this operation, procedures for back-up are included in the software. The mixed integer problem is solved by running all available scenarios and advising the optimal configuration and capacity set-points for the individual units within the defined constraints.

- Dynamic optimization is currently applied only to a very limited extent, for several reasons:
- – Dynamic simulation is currently restricted, and the simulations are mainly applied around a steady-state point for control design and operational studies. The simulations of start-up and shut-downs are subject to a large number of discontinuities which are still difficult to describe in a fundamental way. Discontinuities such as phase changes, filling and emptying of vessels and also trays in columns, reverse and alternating flows, absorption followed by desorption for regeneration, but also in correlations which describe a physical phenomena over large operational ranges.
- – Estimation and prediction of process parameters during operation depend on the technique, but also require a high accuracy of the dynamic model.
- – Simultaneous data reconciliation and parameter estimation in a dynamic environment is commercial not yet available.

Current applications are the optimization of transient trajectories during grade changes in a continuous process, and the optimization of batch cycle times.

Summary project methodology for OO This section provides an overview of project methodology with its activities that will lead to the successful implementation of an OO project. An overview of the overall approach is given in a project methodology flowsheet, see Table 9.2. The essence of each step will be discussed.

- A feasibility study should give a detailed overview of the potentials of an OO project. It will give a technical evaluation as well as an economic overview based on a cost–benefit analysis. The study needs to include time schedule, manpower planning, and an overview of factors which might have an impact on site or company standardization.
- Scope definition must be based on the results of the feasibility study, and clearly define the objectives of the project.

- Development and installation of the performance meter needs to follow the scope of the project and satisfy the accuracy requirements.
- Development of the control structure is an essential element of an OO project as it is based on the assumption of steady-state operation, and emphasizes closed loop operation for BC and MBC. The results of this step are used for the design of the BC and MBC, and the DOFs for MBC and OO are defined.
- Model development needs to be based on an equation-based simulator to achieve rapid solutions. Next to the modeling of the performance of the individual units (including the reactor model(s)), it is especially the description of the constraints that requires attention. During optimization, the process will be pushed against its constraints, and either these constraints are incorporated into a constraint controller or they are calculated and implemented in the model. The parameters are selected preliminarily for the model building; the final selection will be done during model validation. The robustness of the model need to be extensively tested over the operating window.
- Build executive defines the OO operational architecture with all necessary empty steps included. The communication between OO, BC and MBC through a database at BC level must be defined.
- Implementation of data analysis, data reconciliation (including full designed performance meter and the parameter estimation) takes place step by step. In effect, the optimization is taken in operation step by step. During the data analysis step, gross instrument errors are detected, the steady-state situation is observed, and the decision criteria are defined. If steady-state criteria are not satisfied, the control needs to be reconsidered. Ultimately, the performance of the control is verified.
- Implementation of data reconciliation emphasizes the determination of the reconciled mass balances, resulting in determination of gross errors, feed rates and composition, and the reconciled performance measurement. The output of this step starts the DR&PE module.
- Implementation of parameter estimation is initially done in interaction with the model validation step. The parameter estimation will be done simultaneously with data reconciliation of plant measurements (being selected distributed over the process), with the overall process model. The output of this step is summarized in the simulated process performance. A comparison with the reconciled performance measurement should pass a defined criteria, to be used as warning. The parameters ultimately selected for optimization are available for the next processing step.
- Model validation is an essential step in the design of an OO system, but it does not directly play a role in the execution of OO cycle. The validation is done by performing an experimental design program of the DOFs over its operational range. During the tests runs extensive measurements and samples are taken for detailed analysis and fixed parameters are set free for estimation purposes. Now, an extensive off-line study must be performed to evaluate the overall process model over its operational range and search for modeling errors, and update parameters, including those that were fixed. Off-line

optimization exercises provide a good insight into the robustness of the model for optimization. Any problem in this area often requires model updating.

- Implementation of CLO is the last operational step, and concludes the whole sequence of OO, from data analysis to implementation of set-points.
- Evaluate and maintain the project. Specifically, the maintenance of the system is not a trivial effort, and an ongoing maintenance system needs to be set up to maintain the operation and quality of CLO.
- Other types of optimization are discussed briefly, such as off-line optimization, mixed integer optimization, and dynamic optimization.

9.7 Pragmatic Approach to Operation Optimization

Most applications of OO take place in existing processes. Therefore, it is a legitimate question to ask whether the approach taken as described above is the best. If the process is well-known, not only from a reactor kinetics standpoint but also from a process modeling perspective, the size is of a world-scale plant, and the process is subject to frequently changing economic environment, it most likely is. In many plants, the process knowledge is only available to a limited extent and the plant capacities are limited. The approach taken in those situations might be more step-wise. The question will be, "What will be the preferred step plan?". In the first place, the steps planned need to have a value contribution and be sufficient to recover the investment required in knowledge (software) and hardware. The order of steps to be considered are:

- Reactor modeling
- Performance meter
- Process modeling, off-line optimization
- Quality of control, to achieve process stability, including self-optimizing control
- Constraint control
- Process optimization (closed loop)

It is not likely that all these steps have to be taken, and ultimately only one, two or more steps will be required. The order of development is not necessarily as tabulated above, although the logic is in agreement with the order of implementation for total OO. The following qualitative approach is proposed for the selection of implementation steps. The different steps are listed, and are given an effort (investment) in knowledge and potential added value level. Both levels have four categories: High (H), Medium (M), Low (L), and Not Applicable (NA).

The qualification of the different quality levels are:

Reactor model

- **H** is for a kinetic reactor model which includes product distribution and properties like a polymer reactor model or a complex multi-component reaction model (e.g., for cracking of hydrocarbons).
- **M** is for a kinetic reactor model which predicts product distribution (e.g., a styrene reactor model; no product quality involved).
- **L** is for a conversion reactor model (e.g., a hydrogenation reactor), fixed bed or a CSTR type, for full conversion or any model of reasonable quality that can be bought. However, validation might still be an extensive effort which might bring it into the M level (be aware that the models ultimately need to be equation-based in case the source is not made available – at least access to the derivatives is a requirement).
- **NA** is for a polishing reactor (e.g., chemisorption for low impurity levels), not being a constraint nor have any significant contribution to the operational cost.

Performance meter

- **H** In case operation optimization is going to be implemented, to what ever extent off-line or closed loop, a performance meter is a requirement. Its use will not be restricted to performance measurement, but it will also include the necessarily model validation.
- **M** When process stability and constraint control is to be implemented, the meter gives a clear picture of the contribution of these improvements. Operational activities where the number of DOFs for operation are limited in a stabilized process
- **L** When no optimization or control improvements are planned and operational DOFs are restricted.
- **NA**

Process model

- **H** is for complex process plants with many unit operations(over 12), including internal utility generation such as refrigeration (e.g., olefin plants, refineries, propylene oxide/styrene plants, but also smaller plant with multiple unit operations).
- **M** is for medium process plants with 8–12 unit operations (e.g., butadiene extraction plants, hydro dealkylation plants).
- **L** for simple processes with a low number of unit operations (e.g., glycol plants, ethyl-benzene plants), process models which might be bought from technology suppliers, and ultimately need to be equation-based and written for a standard flowsheeter.
- **NA** is for simple units which might be optimized by self-optimizing control. System.

Quality of control

- **H** Process that requires many operator interventions to compensate for disturbances and requires ongoing adjustments to maintain quality operation. The cause might be frequent changes in feedstock rates other external disturbances, and difficult quality control caused by interaction.
- **M** Processes that are less subject to disturbances and interaction, like constant feed composition and major quality loops closed.
- **L** Process only minimal subject to external disturbances and interaction such as constant feed streams and most quality loops closed.
- **NA** Process not impacted by external disturbances and interaction such as total automated unit operations as refrigeration systems.

Constraint operations

- **H** Process is running against different constraints at different units, like capacity constraints and environmental constraints (by processing different feeds, different constraints might become active also constraints at low capacity or changing meteorological conditions).
- **M** Process have a moderate number of constraints, like processes with feed streams with constant composition and those running only incidentally against constraints.
- **L** Process running below capacity and only incidentally forced to an extreme operational regime which also may include low-capacity operation or equipped with constraint controllers on most activated constraints.
- **NA** Almost never running against a constraint or fully provided with constraint controllers. Floating pressure controllers or maximum duty control on a refrigeration system can also be considered as constraint controller next to MIMO controllers.

Note: after implementation of an off-line optimization, constraints become more visible and often there are more constraints than would be noticed without optimization results at hand.

Optimization closed loop

- **H** Processes with many economic disturbances at a frequency of a few times per day, such as processes with wide feed slate and product distributions, a high number of DOFs likely with a large number of units, highly constrained operations which is implicitly coupled to the processing of wide feed and product slates. Parameters that need a regular update.
- **M** Processes with several economic disturbances and a moderate number of DOFs (5–10) on a daily basis.
- **L** Processes with a limited number of disturbances and DOFs (<5) on a less than daily basis, with off-line optimization results available for manual implementation.
- **NA** process with low number of disturbances and DOFs that are already manually implemented based on off-line optimization results.

Note: parameters that need a regular update can only be updated within a closed loop environment. Such a situation always may force the project to an **H** level.

The added value for the above-mentioned steps needs to be determined for the specific situation. This will always remain difficult, for example in off-line optimization. You cannot have a good idea of how far you currently operate from the optimum if the optimum is not known! It is the author's experience that the first off-line optimization results tell you a lot. At first, it tells you where the operational region for optimum operation lies, and it also focuses attention on the constraints. The spin-off will be that it is quite easy to calculate the achievable savings of potential removal of hard constraints.

To illustrate using the above-mentioned qualitative approach, three processes were selected. On an arbitrary basis, the knowledge and added value level of these processes were chosen and presented in Table 9.5. The assumptions made for the different plants were as follows:

- *Olefin plant* has complicated reactor model, a wide variety on feeds and composition, many unit operations, a large number of DOFs, a high frequency of disturbances (several per day), and a very large capacity plant with many constraints.
- *Ethylene glycol plant* has simple reactor model described in literature, single constant quality feed, limited units operations, few DOFs, and limited constraints.
- *Butadiene extraction plant* has no reactor, variable feed composition, medium number of units, medium number of DOFs, frequent (daily) changes in feed rate and composition, not running against constraints.

Table 9.5. Profile of knowledge required and potential added value for OO opportunities of olefins, ethylene glycol and butadiene extraction processes.

	Olefins		***Ethylene glycol***		***Butadiene extraction***	
OO activities	Knowledge	Added Value	Knowledge	Added Value	Knowledge	Added Value
Reactor models	H	H	M	H	NA	NA
Performance meter	H	H	M	M	M	M
Process models Off-line optimization	H	H	M	H	M	H
Stability and quality control	H	H	L	L	H	H
Constraint operations	H	H	L	L	M	L
Optimization closed loop	H	H	L	L	M	M

H is high , M is medium , L is low , NA is not applicable

The results show a profile of these plant regarding OO opportunities. Based on the above arbitrary analysis, one might conclude that the plants are potential candidates for the following implementation OO steps:

- An olefin plant is a candidate for CLO.
- An ethylene glycol plant should have off-line optimization.
- A butadiene extraction plant is a candidate for off-line optimization and a stability and quality control project.

Summary

- A qualitative approach is discussed for the implementation of OO in steps whereby the ultimate CLO is not considered necessarily as the last step.
- The sequential order of the steps are: reactor modeling, performance meter implementation, off-line optimization, quality of control, constraint control, and CLO.

9.8 Appendix

The Optimization Technique based on the Lagrange Multipliers and Analysis of the Result of a Reconciliation of Measurements versus Modeling Results

The Lagrange optimization technique is also used for the minimization of errors during data reconciliation and parameter estimation steps. The analysis of the results is used to develop an estimation of reliability or precision of reconciled values. A mathematical approach is taken by Heyen (1994) to determine analytically the precision of the reconciled values. The same problem could be solved by the application of stochastic technique as a Monte Carlo simulation to calculate the precision. The mathematical technique is of greater value as it also opens the possibility to calculate contribution factors and sensitivity coefficients. The analysis is done by extracting more information from the Jacobian matrix of the constraint equations. Standard deviations for all state variables, measured or not measured, are related to the standard deviation of the measurements.

Mathematical development Optimization is expressed as a constraint minimization problem. The assumption is made that the constraints are linear or linearized.

Notation

X_i	validated measurement	$i = 1,m$
X'_i	measured value	$i = 1,m$
σi	measurement standard deviation	$i = 1,m$
Y_j	unmeasured variable	$j = 1,n$
h_k	constraint equation	$k = 1,p$

Linear constraints are expressed as:

$$AX + BY + C = 0$$

where A is a $(p \times m)$ constant coefficient matrix
B is a $(p \times n)$ constant coefficient matrix
C is a $(p \times 1)$ constant coefficient matrix

The constraint minimization problem is:
min $(X - X')^{T} W (X - X')$
s.t. $AX + BY + C$
with $W = \mathrm{diag}(1/\sigma i^{2})$

The constrained problem can be transformed into an unconstrained one using Lagrange formulation:
min $L = (X - X')^{T} W (X - X') + 2\lambda^{T} (AX + BY + C)$
X,Y, λ
where λ is a $(p \times 1)$ matrix (Lagrange multipliers)
Stationarity conditions are:

$$\left(\frac{dL}{dX}\right) = WX + A^{T}\lambda = W X'$$

$$\left(\frac{dL}{dY}\right) = + B^{T}\lambda = 0$$

$$\left(\frac{dL}{d\lambda}\right) = AX + BY = -C$$

A square matrix is defined (size m + n + p) an array V and an array D

$$M = \begin{vmatrix} W \; 0 \; A^{T} \\ 0 \; 0 \; B^{T} \\ A \; B \; 0 \end{vmatrix}$$

$$V = \begin{vmatrix} X \\ Y \\ \lambda \end{vmatrix} \quad D = 0 \quad \begin{vmatrix} WX' \\ \\ -C \end{vmatrix}$$

The solution of the optimization/validation can be expressed as:
$V = M^{-1} D \; M^{-1}$ is the sensitivity matrix
Both X and Y arrays appears as linear combinations of measured values X'
If we note $N = M^{-1}$ we will have $V = ND$
The sensitivity matrix allows the evaluation of the validated values of a variable from all measured variables

$$X_i = \sum_{j=1}^{m+n+p} (N)_{i,\,j}\, D_j = \sum_{j=1}^{m} N_{i,\,j} W_{jj} X'_j - \sum_{k=1}^{p} N_{i,\,n+m+k} C_k$$

$$Y_i = \sum_{j=1}^{m+n+p} N_{n+i,\,j} D_j = \sum_{j=1}^{m} N_{n+i,\,j} W_{j,\,j} X'_j - \sum_{k=1}^{p} N_{n+i,\,n+m+k} C_k$$

The variance of a linear combination Z of several variables X_j is known from literature,

$$Z = \sum_{j=1}^{m} a_j X_j \quad \mathrm{Var}\,(Z) = \sum_{j=1}^{m} a_j^2 (X_j)$$

The4 following variance of the validated measured variables are obtained:

$$\text{var}\ (\text{X}_\text{i}) = \sum_{j=1}^{m} (N_{i,j} W_{j,j})^2 (X_j')$$

for the estimated unmeasured variables:

$$\text{var}\ (\text{Y}_\text{i}) = \sum_{j=1}^{m} (N_{n+i,j} W_{j,j})^2 (X_j')$$

Taking into account:

$$\text{var}\ (\text{X}'_\text{j}) = 1/\ \text{W}_{\text{j j}}$$

now:

$$\text{var}\ (\text{X}_\text{i}) = \sum_{j=1}^{m} N_{i,j}^2 / (X_j')$$

$$\text{var}\ (\text{Y}_\text{i}) = \sum_{j=1}^{M} N_{n+i,j}^2 / \text{var}(\text{X}'_\text{j})$$

The contribution of the variance of measurement k in the estimation of the variance of reconciled state variable i is derived from the equation above:

$$\text{Contribution}_{\text{k,i}} = \left(\frac{\text{var}(\text{X}_\text{i})\text{var}(\text{X}'_\text{k})}{(M^{-1})i,\ k^2} \right)$$

The sensitivity coefficient relating the validated variable to the measured value and the standard deviation are:

$$\text{DerVal}_{\text{k,i}} = \left(\frac{dX_k}{dX_i} \right)\ \text{DerAcc}_{\text{k,i}} = \left(\frac{dX_k}{d\sigma_i} \right)$$

The analysis technique to determine the accuracy of the reconciled data has been developed by Heyen (1994) and further extended by Heyen et al. (1996).

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Chapter 10
The Efficient Design and Continuous Improvement of High-quality Process Plants from an Organizational Perspective

10.1
Introduction

The challenge is to design and operate high-quality competitive process plants, and the application of design philosophies and techniques is discussed in this chapter. The intention is to describe briefly a method of achieving the design of simple and robust process plants. The method is not intended to be a rigid frame work, but simply a guide to how this might be approached. The method is based on practices of several companies who implement this in their own way, following within-company procedures.

A differentiation is made in improvements for an operational process versus design projects; in the latter case, revamps as well as new facilities must be considered.

The *continuous improvement of a high-quality plant* demands four types of activities in order to ensure long-term optimal process performance. These activities concern the following questions:

- How do we maximize the capacity of the process plant?
- How do we upgrade the reliability and availability of the process?
- How is the quality of the operation upgraded?
- How do we achieve optimal operation of the process plant?
- How can we determine design opportunities?

The design of a high quality plants is based on the design philosophies, and the techniques as discussed require a structural approach. This must be valid for revamps as well as new facilities. The main objectives for a project are: to stay within budget; in time; and at low engineering cost. In general, these are the objectives for a project manager assigned to build the plant. Another objective – which is of similar importance – is to build a competitive plant that is able to compete with other plants over its life time. The approach taken to achieve a high-quality plant includes two aspects:

1. The work process covering for process design, engineering, construction and start-up of the process.
2. The quality of the design.

The work process concentrates on the organizational aspects of the design process. It defines what should be done, in what order it needs to be done, and which disciplines need to be involved. The quality aspects are concerned with how these activities are performed to achieve a quality result regarding process performance.

The aspects of continuous improvement of a process plant and the efficient design are discussed in this chapter.

10.2
Continuous Improvement of a High-quality Plant

In today's global markets, it is competition that forces process plants to stay competitive. Presently, a plant needs to be – and remain – competitive, more than in the past where markets were more local and often protected. Therefore, on-going activities are necessary to improve the plant performance (Bascur and Kennedy, 1996). These improvements can be achieved in different areas, and include:

- Process capacity performance
- Process reliability and availability
- Quality of operation
- Optimal operation
- Opportunities for design improvements.

Each area demands a specific approach, which is discussed in the following subsection.

10.2.1
Process Capacity Performance

From the early days of its operation, the performance of a production plant is measured in terms of cost, capacity (if applicable for more products), raw material and utility utilization, expressed in unit ratios. The frequency of the measurements was increased over time, most companies perform such monitoring on a daily basis. An exception is that of the cost calculations which, depending on the company, are executed on a weekly, monthly, or even quarterly basis. Due to severe competition, one currently has to up-grade performance on a continuous basis. Therefore, more and different measurements are required, and these generate the stimulation to improve production. Realistic target setting is a proven methodology to realize this latter effect. Bench-marking also offers a means of measuring, as well as a stimulation to upgrade performance (Ahmad and Benson, 1999).

The process capacity performance measurement is an additional instrument to measure process capacity expressed in terms of capacity at quality, over fixed time periods. The capacity performance limitations are divided into categories, to register causes of deviations from its maximum demonstrated capacity. For example, the categories for a lower than demonstrated capacity might be:

- market demand,
- mechanical failures,
- process failures,
- process availability (regeneration, shut-down),
- equipment availability in multi-purpose usage,
- logistic constraints,
- low quality performance.

The measurement results show not only the capacity gaps but also the opportunity gaps for improvements under the different categories. It will be clear that the targets for these gaps need to approach zero. The approach for these opportunities will be discussed below. The logistic and business opportunities are excluded, as these are not a production plant responsibility.

10.2.2
Process Reliability and Availability

Plant reliability and availability (Bascur et al., 1997) can be divided into the process and mechanical causes for production loss. Process, as well as mechanical, causes need to be analyzed for: grass root causes; common causes and frequencies of occurrence on similar items (pumps, temperature measurements, fouling, etc.); mean time to repair (MTTR); mean times to stop and recover production; and production losses.

The analysis of the process failures/losses (a lower production rate due to process reasons also falls under this category) might be done in concert with research. Typical causes for process failures/outages/losses are:

- fouling,
- regeneration of catalyst,
- cleaning or washing steps,
- sterilization,
- product changes.

The opportunities need to be quantified money-wise. Multiple functional thinking needs to be applied to generate creative economic solutions or areas for further investigations. The solution of these types of problem is time-consuming, but they often have short pay-back times.

Mechanical failures are easier to recognize, but it is more difficult to find the root cause. The investigators often have a traditional maintenance background and so have a tendency to blame the equipment and repair it (Figure 10.1). A good approach is to appoint a production engineer for the grass root analysis, but to have maintenance and process engineering experts in the team. The analysis emphasizes the same elements as mentioned above, but it will contain some additional elements

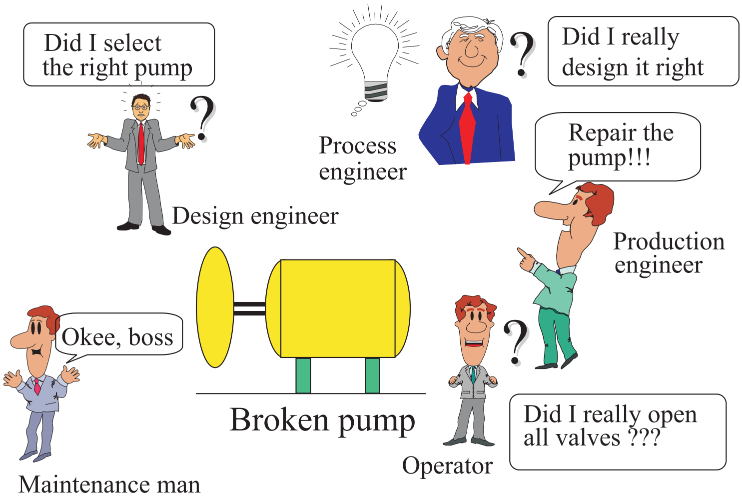


Fig. 10.1. Broken pump,for the third time.

typical for mechanical failures. Failure rates have different distributions modes, including normal, log-normal, Poisson, exponential, and Weibull (for details, see **Chapter 6**). Failure rates are collected and put in a reliability database under its component family with its specific component attributes. The data from one plant can be compared with reliability databases that are open to the public domain (CCPS, 1989; Oreda, 1992) and vendor data. The failure distributions are often used for predictive maintenance programs. The evaluation and the solution to the mechanical failures often have to be discussed with detailed engineering, and with the suppliers of the equipment. The latter often develop equipment improvements (this is in their best interest).

The above-mentioned grass root analysis and improvements of reliability and availability are activities that need to be ongoing.

10.2.3
Quality of Operation

Most instrumentation systems have an event-tracking option. The event tracking mechanism is the best way to analyze the events of process units. The objective of the analysis is to determine what kind of actions must be taken to operate the unit, the events being divided into:

- Alarms coming in, and its subsequent actions.
- Operational actions as step actions to move units into another operational step.
- Control actions to overcome interaction and reject disturbances.
- Supervisory actions feed changes or product changes.

The objective of simple and robust plant is hands-off operation. The analysis of the events is to identify the areas for improvement of control and operational software to reduce operator intervention. The same type of analysis can be applied for field operation; in that particular case the operator's activities must be registered as manual and analyzed for improvements.

The described activities should lead to an inventory of potential process improvements to achieve simple and robust operation. The event-tracking must be a daily activity of the day supervisor, watching for problems and opportunities to keep the operation simple and robust.

10.2.4
Optimal Operation

For optimal operation we need two different tools: a continuous plant performance measurement (profit meter); and an optimization model.

The profit-meter (see Krist et al., 1994) is a technique to measure plant performance continuously (for details, see **Chapter 9**). It is based on the principle of mass balance reconciliation of the process streams, within and at the boundaries of the plant. Multiplication of the reconciled mass and energy flows with its economic value gives an on-line money-wise performance picture of the operation (Figure 10.2). Any plant that wishes to optimize its operation needs a performance measurement as a profit meter. The type of profit meter will depend on the application and its design, although different types of profit meters might run at the same time.

In its most elementary form, the operator might use it at fixed conditions as, feed composition and prices. In this concept, he/she can watch the plant performance and anticipate on the impact of his/her own manipulation.

Optimization models for either scheduling, off-line or closed loop optimization are further tools for performance improvement. The validation and the maintenance of these models over the operating range of the process are a major production concern.

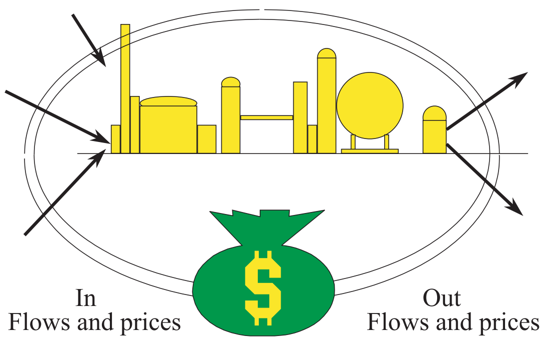


Fig. 10.2. Profit meter.

A non-validated model is useless for optimization. A good method for validation of off-line models is to compare the simulated results with the profit meter results. Adjustments of process parameters or model updating are the degrees of freedoms to achieve a closer match between plant data and simulated data. The use of off-line models is limited to situations that are not subject to frequent variations, less than once per day while process parameters do not change during operation. Closed loop optimizations must be provided with an on-line profit meter and an integrated data reconciliation and parameter estimation module to keep the models valid (see **Chapter 9**).

Operation optimization pushes a plant against its constraints, and shows opportunities for improvements. The capacity constraints at environmental conditions are challenges to operate with maximum variable throughput by taking advantage of the day and night temperature cycle for capacity maximization.

Summarizing, production should in order to optimize production:

- Install a performance meter on the process, and utilize optimization models for operation.
- Validate and maintain the optimization models.
- Monitor the process for operational improvements with as reference the performance meter.
- Identify constraints and search for ways to eliminate these.

10.2.5
Opportunities for Design Improvements

The results of the above activities already should give the production and process engineers/managers some insight into the potential(s) for design improvements. Opportunities for capacity improvement might be concluded from the process capacity performance. Analysis of the data and simulation results will show restrictions on capacity, such as valves, heat exchangers at environmental extreme conditions, or others.

Operation optimization results push the process conditions against constraints. This information is also valuable as de-bottle-necking information. Plant designs are often based on arbitrary decisions on specifications for recycle streams, while operation optimizations show the direction that these must take. Design optimizations should provide the ultimate answer.

Reliability and availability studies are other valuable input data for improvements. The identification of reliable components, or improvements in less reliable components, might lead to single components in a revamp, or to a new facility. On one occasion, a situation was noticed where a compressor was spared and the equipment was regularly utilized for back-up. The challenge was to analyze the compressor failures in detail and solve these to remove the spare compressor. In case supervision does not take the decision to remove a spare unit, the remaining one will never achieve the required reliability.

Logistic management has the opportunity to build up experience with just-in-time production to reduce storage and its facilities. Existing plants can benefit from these opportunities to reduce working capital, and give the storage facilities another destination.

Summary

Continuous improvements of plants require on going performance tracking and activities to realize progress. The area's requiring specific attention are; capacity, reliability, quality of operation, operation optimization, design improvements.

- Capacity improvements are achieved by systematically identification and evaluation of constraints in the area of; market, logistics, plant availability and reliability – mechanical as well as process wise –, product quality.
- Reliability improvements ask for grass root analysis of failures including planned process outages and proposals for improvements
- Quality of operation based on the concept of hands-off operation requires analysis of all operation manipulations on the panel and in the field, and evaluation for improvements.
- Operation optimization are achievable by installation of a performance (profit) meter and optimization models for; scheduling, off / closed loop optimization.
- Incremental design improvements can be easily identified with optimization models as these push operation against its constraints, and incremental opportunities can be quantified by elimination of selected constraints.

10.3 The Design of High-quality Plants

During the last decade, many challenges have arisen within the engineering environment, but these can be grouped into three different challenges:

1. The design of low-cost and high-quality chemical plants, at design capacity.
2. Build and engineer the facility within planned cost (budget), on time and with a demonstrated 100% capacity within a few months after start-up.
3. Design and engineer the facility at low cost and in a short time period.

The *low cost of a high-quality plant* is specifically addressing the capital cost. It has been shown that the capital of a plant, including its logistics, can be reduced by 30% compared with conventional designs by the application of simple and robust design principles (see **Chapter 3**) (Koolen, 1998).

The *quality of a plant* is of crucial importance, especially when we realize that the lifetime is somewhere between 20 and 40 years for a basic chemical plant. Under quality, we understand a high-performance plant with respect to selectivity and unit ratios, reliability, safety, environmental compliance and ease of operation. Such a plant is also called a *competitive process*. The realization of the quality aspects within a design must deal with many details that need to be incorporated during the design.

Engineering and constructing a plant within budget and on time is mainly dominated by the project definition, as was concluded by Independent Process Analysis Inc. (Merrow and Yarossi, 1994), not forgetting that the engineering and construction of the facility has to meet certain standards.

Design and engineering at low cost has initially to do with the working methods – often called the work processes. During the design, we must apply the concurrent engineering concept to meet short project delivery times. The design of such a work process and its validation is of crucial importance (Rummler and Brache, 1995).

The above-mentioned opportunities for the chemical industry are addressed from two perspectives (Koolen, 1999):

1. An organizational perspective by introduction of a consistent work process.
2. A quality perspective by application of value improving practices during the design.

The development of an efficient work process is fundamental. A feed-forward organizational concept has to be incorporated in the work process to avoid or minimize rework from either the businesses or the involved functions.

The objective to design the work process is to enable a *no-change mentality*. It will be no surprise that concurrent engineering is an element that is an important facet of an efficient work process, particularly so (as that aspect is recognized) to improve the efficiency of design and engineering (Prasad, 1996). The completeness of the design before detailed engineering starts (called front-end loading) is another important aspect of the work process. This will improve engineering and construction of a facility from a cost and timing perspective.

The performance of the work process is verified through external bench-marking with experienced companies that have a long history in the project evaluation of chemical plants.

The quality aspects of the process plant will be discussed. A concept is developed within the chemical industry that addresses different aspects of quality. The terminology *value improving practices* (VIPs) has been introduced. The different quality aspects are explained, along with the best place for implementation in the work process. Introduction of the elements of quality in the design work process is seen as essential for a quality design process.

10.3.1 Work Processes

A work process appears similar to the operation of a production plant. In a production facility, a step-wise set of physical operations is executed to produce a certain product from a raw material. In a work process, a step-wise set of organizational operations (activities) are executed to deliver a certain service (product) based on starting conditions (raw material).

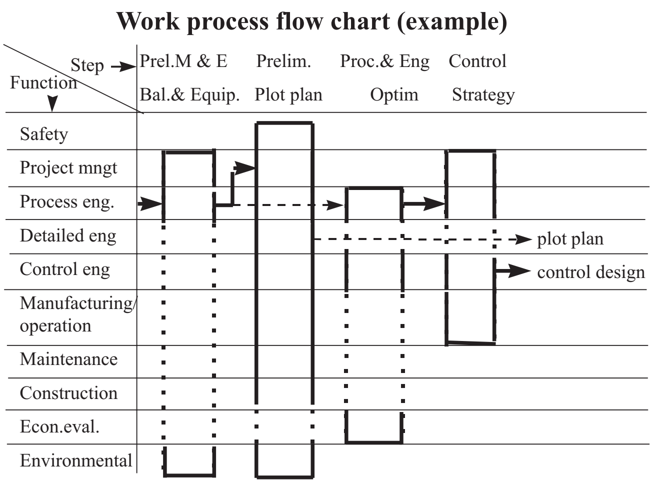
Several reasons can be recognized that lead to the desire to implement work processes. Drivers that play a role in the development of work processes are:

- The desire to work with fewer people goes hand in hand with less organizational layers and more empowerment, but within a well-defined organizational framework. This is one of the main reasons why work processes are extensively introduced.
- Logistical spread design work places, where we need to communicate uniformly and quickly.
- Automation of project organization requires consistent working methods for a structural approach.
- Quality processes also demand for structured well-documented approaches.

In industry, as well as in (semi)governmental organizations such as healthcare, all kinds of work processes are (or have been) developed to improve efficiency of operation.

Work process formats have been developed among others by Rummler and Brache (1988, 1995). An organizational map, as used in this report, shows a flow diagram in table format that shows the steps to follow horizontally, and the functions vertically. The functions are all represented, from business to operations. The involvement of a function in a step is shown as solid vertical lines (for an example, see Table 10.1) A flow-line connects these steps. The initiator for each step is assigned and recognized by the inlet arrow of the step. The main responsible function for a step is recognized by the position where the flow-line leaves the step. Each step has a description that defines the objective, the input requirements, and the output of the

Table 10.1. Work process flow chart (example).



step, the main functions involved, and its responsibility in the step. It also contains references such as company procedures. An example of a short step-wise description for the development of a plot plan for a new facility is shown in the Appendix 10.1.

Decision and review steps are part of the work process. The reviews are technical as well as organizational A good work process is a feed-forward controlled concept with feed-back loops built in (In't Veld, 1985) (Figure 10.3). This says that the work process needs to capture up-front activities or procedures to avoid rework from the reviews. The overall concept is: "do things right the first time".

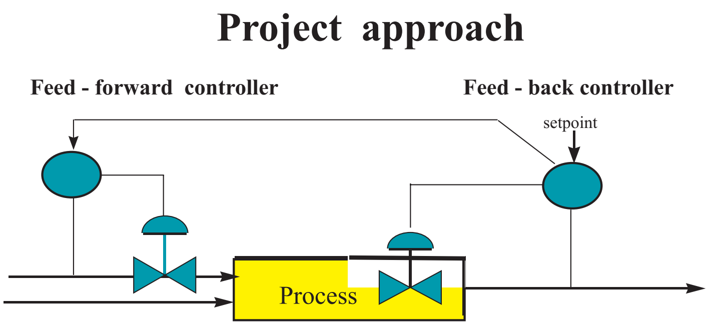


Fig. 10.3. An efficient controlled process has a feed-forward controller with a feed-back adjustment.

10.3.1.1 **The development of a work process**

The development of a work process (WP) needs to follow a set of rules to assure the quality of the work. The development team needs to have the following key elements:

- Scope of work
- Development methodology
- Independent moderator
- Highly qualified members of all functions involved. All functions involved should be represented by highly qualified people; (it might be worthwhile to introduce external company representatives during the development if they play a role in the work process).

Some key words for people involved in the development are: open minded, with a mandate for decision; and respect for each other.

A fully developed WP should have as end result:

- Flow diagram
- Step descriptions
- Owner assigned
- Maintenance system

Some *generic aspects* that are important to be recognized for the work process development team are:

- Reviews are the feed-back mechanism for the process, and there is no replacement for this, although (as stated before) it is preferable to do things right the first time. Therefore, it has to be considered to include references to specific procedures in the work process documentation. In this way the project team can anticipate beforehand and avoid rework (feed-forward versus feedback).
- Bench-marking. The work process is essential for the competitive operation of a company. Therefore, it will be useful to compare the operational results of the critical work processes with an external bench-marking.

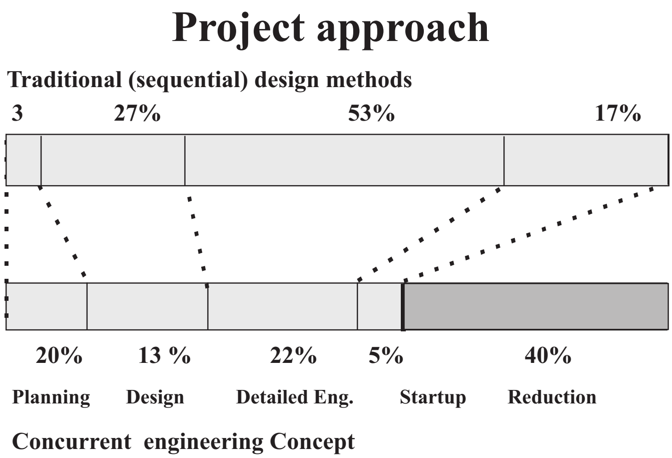


Fig. 10.4. Concurrent engineering time reduction (Ref: Prasad '96).

10.3.1.2 **Work process for capital projects**

Aspects that are specific for capital projects are:

- Apply concurrent engineering versus sequential; this will result in less recycle of work and faster projects (Figure 10.4) (Prasad, 1996).
- Functions to be represented in the team are: business, project management, process engineering, control engineering, plant operation, project engineering, design engineering, project control (estimating and planning), construction, maintenance, procurement, economic evaluation, environmental health and safety.
- A capital project should apply the best technology but it has constraints on:
- – timing – the time available for developments is restricted.

– technical risks – there are limits on the implementation of new designs or techniques. In general, limited incremental developments are applied on current technology to reduce the technical and related business risks.
- The quality of a project is only partly covered in a WP.

A work process defines:

– *What* should be done.
– *When* it should be done.
– *Who* should do it.
– *Which* procedure should be followed.

However, a work process does not indicate "*how*" to do it, in as much as it is not covered in a procedure. The quality aspects of the design will be covered later in this chapter, under "Value-improving practices".

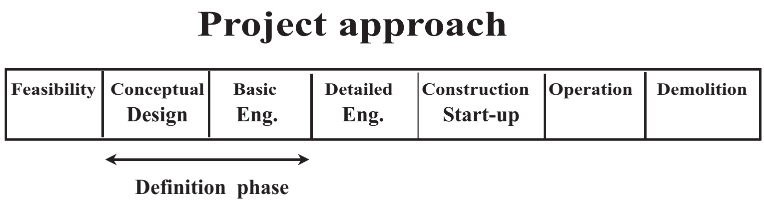


Fig. 10.5. Life span of a project.

10.3.1.3 **Project phases**

A project is in general executed in a number of phases (Figure 10.5):

- Feasibility
- Definition often this phase is split in two parts:
– Conceptual design
– Basic engineering
- Detailed engineering
- Construction.
- Operation and evaluation.
- Demolition

The descriptions of the steps and the functions will be different for among companies, as each company will have its own work process and different functions and responsibilities (although such variations will not be large).

Remarks The definition phase is often divided in two phases: conceptual design; and basic engineering. The overall differences are in the level of completeness.

- In *conceptual design*, the emphasis is on mass and energy balances, control diagrams showing all instruments hooked up to the control system (in a simplified notation) including basic control loops, and preliminary equipment sizing for cost estimation only, preliminary plot plan and equipment layout.
- *Basic engineering* includes P&IDs for process as well as utilities, equipment specifications for engineering, piping specifications, process data for piping and instruments, final plot plan and equipment layout.

Conceptual design has a lower level of definition, and therefore has a less accurate estimate. The advantage is that the business does not spend all the cost for the preparation of a full definition package while they have other business options under evaluation. Another advantage is that basic engineering can easily be carried out externally on a conceptual design package The disadvantage is that the company loses time in the preparation for this additional phase and its decision steps.

As discussed previously, the efficiency in engineering (speed and cost) is realized by the application of a work process that incorporates the functions at the right time to prevent rework.

10.3.1.4 **Bench-marking**

A work process can be judged by the evaluation of project executions with external evaluators. External bench-marking has the benefit that it not only shows your own performance, but also your relative position to other companies. A generic report on bench-marking was made by Ahmad and Benson (1999). Companies active in this field are the well-known Solomon studies for technology comparisons. A commercial company that has long experience in project evaluation of chemical plants is Independent Project Analysis Inc. (I.P.A. Inc.), who initially gained experience in project evaluation by performing specific studies to explore the reasons behind project failures. Later, they started evaluating different projects in the process industry for a wide range of processes. During these evaluations they collected project information over the total project lifetime from the start of the project until full capacity was realized. This information was ordered and collected in a knowledge database, with which I.P.A. Inc. have developed correlation's between elements of design and project results.

The project results were measured in terms of capital and timing realized versus budget and time plan. They also record the time needed to reach full capacity after construction. Other results measured were design and engineering time. Different elements of design information were collected through answers on questionnaires which were evolving over time.

The ultimate conclusion, found through a parametric statistical technique, was that there exists a strong correlation between the completeness of the design before engineering starts and the project result (Merrow and Yarossi, 1994). Based on this information, the term *front end loading* (FEL) was introduced, which expresses the level of completeness of the design in a number before engineering starts. The effect of FEL versus relative capital cost is shown in Figure 10.6.

In conclusion is can be said the an effective work process includes front end loading, a well defined design basis for engineering and is based on a feed forward approach with feed back (reviews) adjustment to support concurrent engineering

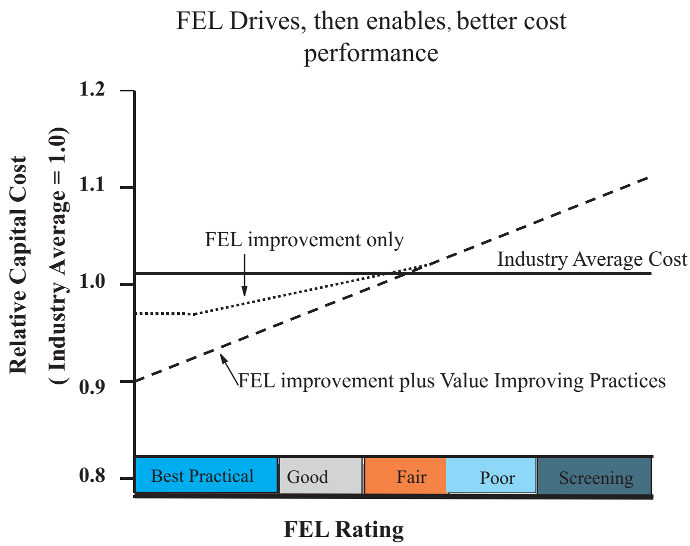


Fig. 10.6. Project approach (Source IPA Inc.).

resulting in a efficient and timely engineering and construction. The effectiveness of the work process can be evaluated by external bench-marking of work process and executed projects.

10.3.2
Quality Aspects of a Design: VIPs

A developed work process does not tell much about the quality of the process design, the exception being those items which must follow detailed quality company procedures, such as safety. To address the quality aspects, the process industry introduced value improving practices (VIP). A VIP being defined as a methodology for a defined set of specific design activities to add value to a project. A list of these VIPs is given in Table 10.2.

The VIPs can be compared with the quality factors of a consolidated list of Herder and Weijnen (1998) (Table 10.3). (The quality factors according the quality of the design process were excluded, and others were regrouped.)

A difference between the quality aspects as presented in Tables 10.2 and 3 is that the industry does not mention safety, and operability. An explanation is that the process industry accepts these items as being well-covered in the WPs or in company procedures, while their fitness for the purpose should be the result of the application of VIPs. Another difference is that items such as process simplification, process/energy optimization, and construction are not mentioned in the list provided by Herder (1999).

The concept of VIPs is also part of the evaluation of I.P.A. Inc. The potential to impact value of VIPs is presented in Figure 10.7, from which it can be concluded

Table 10.2. Value improving practices

Technology selection
Classes of plant quality
Waste minimization
Process simplification
Process/energy optimization
Design to capacity
Reliability modeling
Standardization
Maintenance
Construction

Table 10.3. Quality factors (Herder and Weijnen, 1998).

Safety
Fit for purpose
Performance on raw material / product
Environmental
Control of product quality
Operability
Reliability
Maintenance
Value engineering

that the impact of the value of these VIPs has a ranking order that starts at technology selection and ends with construction. The added value of the VIPs is also illustrated in Figure 10.6.

Below, the individual VIPs are described briefly, followed by the implementation in the work process. The VIP, Classes of Plant Quality and Standardization are not discussed. Classes of Plant Quality mainly addresses the scope of the project, that should be in agreement with the business and based on economics. Standardization addresses the standards of the facility in relation to company standards, the latter often being too expensive.

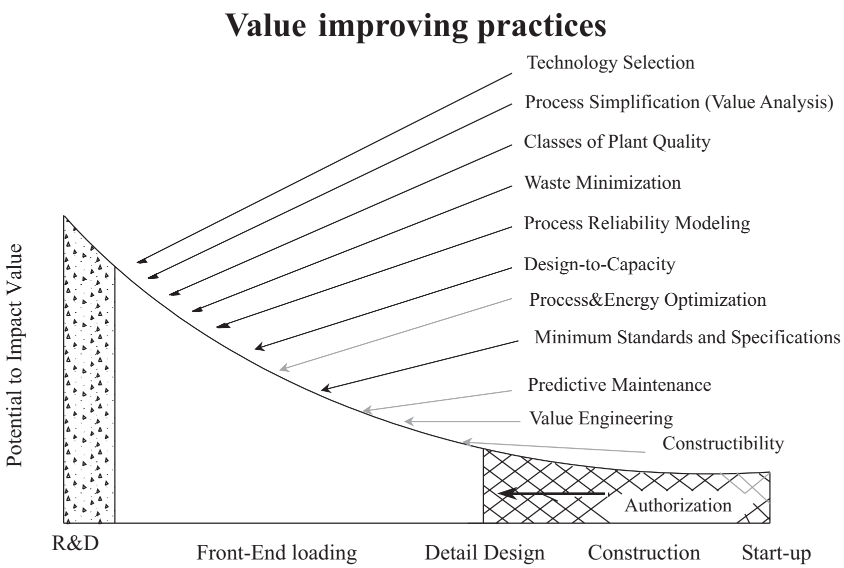


Fig. 10.7. Impact of Value Improving Practices (VIPs) (Source IPA Inc.).

10.3.2.1 Technology selection

Technology selection is a formal process to select the best technology for a competitive plant. The selection should be done by a highly qualified team, which should include process researchers, among other functions. The selection should be done on all technologies (both internally and externally), even if a particular technology cannot be licensed. The selection should include the economics as well as environmental aspects. External bench-marking can be done with a company such as Solomon Associates Inc. Before the final selection is made, a patent search needs to confirm if a certain technology may be applied at the location under consideration. The technology selection will be of crucial importance for the long-term success of the project.

Timing/documentation: the selection is made during the feasibility phase, and documented in the basis for design.

10.3.2.2 Waste minimization

The objective is to reduce the waste stream and its environmental impact on the facilities. Under environmental impact we must consider not only air, water and soil pollution and off-site waste disposal, but also risks to the environment and nuisances such as noise, and sky-line pollution such as flares, plumes and tall constructions. The priorities for reduction are:

- Prevention or reduction of waste production.
- Recycle or reuse of waste material internal or external of the facility.
- Treatment of waste streams (also called “end of pipe” treatment).

Quantified environmental studies are subject to preparation during each phase of the project from feasibility phase to demolition. The content of these studies should have the following elements:

- The environmental requirements (internal as well as external) should be inventoried and considered as mandatory. It would be wise to be prepared for more severe requirements in case the local requirements are not yet at western world standard. Be prepared that there is an ongoing evolution to more severe global requirements.
- The studies should include an environmental balance, not only for the treatment of the continuous waste streams but also for the final rest streams in water and air. It should also include the waste solids and its final treatment and disposal, periodic wastes such as spent catalyst, plant-fouling materials, regeneration waste, and demolishing materials. Be aware that the continuous process will always be subject to variations that may result in fluctuations in the waste streams and its concentration.
- Evaluations of alternatives are required for good decision making, and also for the authorities. The application of the best practical means is mostly used as reference for the authorities.

- The environmental risks need to be determined for emergency situations, and provisions such as emergency ponds need to be addressed. In case dangerous goods need to be transported, transportation risk studies with different modes of transportation and routes might be a requirement.
- All environmental issues are critical for the public, and demand an open, honest, and timely communication. A communication plan for environmental issues needs to be available in the operational phase.

Remarks Sustainability is demanding for more attention. The requirements regarding the efficiency of the process and requirement for Life Cycle Analysis (LCAs) are growing. The LCAs are mostly carried out for product chains, and in general are (in most organizations) a business responsibility. The demand for efficient processes will have to be addressed during the technology selection.

Shortage of water is not seen as a generic environmental issue, but might be a specific local problem. In the last case it has to be addressed in the environmental report.

For an example, see the 10 steps environmental procedure and reviews of Kraft (1992).

Timing/documentation: during all project phases and documented in environmental reports.

10.3.2.3 **Process simplification**

A structured brainstorming session should be conducted to achieve capital and operational savings of the facility. The application of such an approach in process design is quite recent, and fits in the realization of World Class Manufacturing (WCM) (Schonberger, 1986) and Simple and Robust plant designs (Koolen, 1998). The focus is on the process itself, its units and its equipment. This in contradiction to value engineering that is based on the same technique, but generally speaking concentrates more on equipment and its details. For detailed information on value engineering techniques, which are similar for simplification, contact SAVE International (see Reference list for details).

The brainstorming sessions should capture the following elements:

- Information collection; for a facility we need a project scope, index flowsheet, process description, mass and energy balances and any logistic requirements.
- A team with a independent moderator and qualified team members from R&D, process engineering, process control, design engineering, production, project team, business and licenser representatives.
- Creation of ideas is the crucial step. This is done with a technique called function analysis (see Appendix 10.2) (Snodgrass and Kasi, 1986; SAVE International). The opportunity is to create ideas about project alternatives, and that requires an out-of-the-box thinking environment.

- The ideas need to pass a first evaluation, to make a prioritized list of the ideas based on potential benefits and to select the most promising ones for further development.
- Reporting of brainstorming results.
- Development and selection for implementation of promising ideas by the project team.
- Implementation.

Leading questions to create the overall mind are formulated from different perspectives: general, simple and robust plant design, world class plants, environmental and inherent safer chemical process principles (CCPS, 1996; Kletz,1991). The moderator leads the session by going step-wise through the process, and stimulates the discussion.

General points

- Do we really need this process, unit, equipment, utility? Does it add value for the customer?
- Can we replace this functionality with an external service? Services can be bought from an outside companies like; power, steam, water, refrigeration cooling, cooling water, oxygen, process streams, waste water treatment.
- Can we avoid steps in the process were we increase a stream to a higher energy level, such as temperature, pressure or concentration level, decrease it and increase it again? (For the "do, undo and redo" discussion, see **Chapter 5**).

Simple and robust plant design

- Do we design for single robust components? (components might be a processing train, unit, equipment, line, instrument, valve, power cable, etc.).
- Can we combine this process step/equipment with another step/equipment?
- Is the design based on *first-pass prime*?

World Class Manufacturing

- Does the design apply for Total Quality Control? *Do it right the first time*.
- Is the principle of *just in time production* followed?
- Do we consider predictive maintenance?

Environmental

- Can we prevent or reduce this waste stream?
- Can the external risks be prevented or minimized?

Inherent safer chemical process principles

- Can we *minimize* the hazards (less material)?
- Can we *substitute* a material with a less hazardous substance?
- Can less hazardous situations be created through *moderation*, such as less severe conditions, less hazardous form of materials?
- Can we *simplify* the design for operation, minimize direct interactions between different sections?

Timing/documentation: The brainstorming session results need to be documented by the team, the ideas selected for further development, and implementation needs to be reported by the project team. The process simplification is done at the beginning of the conceptual design with the first-pass mass balances available.

10.3.2.4 Process and energy optimization

The objective of the VIP is to optimize the design of a facility as a trade-off between capital and operational costs. This VIP was originally limited to energy optimization, but has been extended with process optimization. The reason is that the impact of process optimization on an efficient design is much larger than from energy optimization alone. Historically, the situation can be explained, the technique for energy optimization with its pinch approach was developed immediately after the energy crisis at the end of the 1970s. The technique for design optimization is industrially (in all practicality) applied at the turn of the century.

Optimization of design has, in comparison to operation optimization, a much larger number of degrees of freedom. Designers want to understand the pathway of process decisions, and therefore plant optimization for design is split into different layers (see **Chapter 4**). The layers to be mentioned are:process synthesis; optimization of consolidated flowsheet including energy optimization. In the long term, there will be developments in commercial software to make integration of these different optimization levels possible. However, many practical problems will remain to be overcome before process designers apply this technique with full confidence of their designs. Remember the process simplification effort which is still at the beginning of an evolutionary state. In a full design optimization model, a large expert system needs to be available to generate all feasible alternatives. Some time will pass before that is realized. For revamps – which still represent the majority of the projects – this will certainly not be solved in the short term. There is no doubt that, ultimately, there will be developments to combine the integration of these optimizations levels.

Conceptual design optimization or process synthesis

As the word says, this must be carried out during the conceptual design. It might be performed by evaluation, optimization, of different cases against the objective function. An alternative way is to describe it as a mixed integer problem based on a super structure with its constraints. In **Chapter 4**, this level was split over two synthesis steps, the final result being an overall flow diagram with the type of separations with its sequence selected and preliminary mass balance – called a "consolidated flowsheet".

Optimization of consolidated flowsheet

The overall flowsheet has been fixed, but the pressure levels, the specification of recycles, and reactor optimal design point are still free, as are the equipment dimensions. The techniques applied are mixed integer or continuous optimizations. The methodology for continuous flowsheet optimization is described by Koolen et al.

(1999). The final result will be a preliminary mass and energy balance based on the consolidated flow diagram.

Energy optimization

This is done based on the preliminary mass and energy balance. A pinch study is started to determine the energy targets (heating and cooling). This must be done within the identified constraints for heat exchange, such as operability, controllability, and safety. Based on these target data, iterations will take place between flowsheet optimization and energy optimization. The final result will be a consolidated mass and energy balance, the energy levels are selected and the major equipment dimensions fixed, such as number of trays, column diameter, and number of compressor stages. Next, the energy network can be optimized, resulting in the sizing of the heat exchangers.

Timing and documentation: conceptual design optimization needs to be done during process synthesis. Optimization of the consolidated flowsheet in interaction with energy optimization are planned after the process synthesis, with the exception of heat exchanger network optimization, which can be done during basic engineering. All the optimization work needs to be documented, especially with its objective functions, its price sets, constraints and the degrees of freedom for the optimization and its sensitivities.

10.3.2.5 Reliability modeling

This is a fairly young applied design technique – excluding nuclear and aircraft industries – to improve process design and to quantify the availability of the process, including its infrastructure (Henley and Kumamoto, 1981&1992), It can generate a ranking of the elements contributing to plant unavailability and its down time due to mechanical failures.

The objective of reliability modeling is based on a quantitative technique; to calculate plant availability, identification of unreliable components, and to provide a tool to optimize the design by the evaluation of design alternatives. The design philosophy, "Design for single components unless, economically or safety wise justified", requires reliability modeling to justify any deviation from single components (Koolen, 1998). The design options for consideration are in order of priority:

- Can we eliminate this component?
- In case of failure, does that necessarily end in a process stop, and in case it does not, can a component failure be survived within its repair time?
- Can we replace this component with a more reliable one?
- Consider redundancy

The technique has been applied both extensively and successfully in the power industry, as well as off-shore explorations (Shor and Griffin, 1991).

Timing: during the conceptual design and basic engineering phase.

Documentation: results have to be documented in a reliability report.

10.3.2.6 Design to capacity

The objective is to avoid unnecessary accumulation of over-design, safety factors and design allowances to prevent high cost. We can differentiate different types of over-design, which as such might be defendable, but the combination of these factors will lead to high cost.

Let us give an example of accumulation of over- design. For the equipment design of a process plant, the hourly mass balance is taken as the basis. The mass balance is often considered as to be fulfilled at the most extreme feed and product conditions on a hot summer's day afternoon, and also for a very cold night in the winter. The end-of-run conditions of the reactor and the maximum fouling will also be additive factors used for equipment sizing. The designer must also have some concern about the physical properties, and he/she will add some "fat" for compensation. However, he/she must also be concerned about the calculation method, with its reference data. So, for a distillation column, they may design at 50% of the required product specification, and at 60–70% of flooding, under extreme conditions. They will most likely size the heat exchangers some 10% above the required area at extreme environmental conditions. This example is a reality in many cases, and that is why a plant can easily have 20% excess capacity in its equipment. This capacity shows up after start-up, when the size of some control valves is increased (this often being the first bottleneck). No consideration is made as to the excess capacity required by the business for future expansion as over-design, although it should be documented within the scope of the project.

The different types of over-design to be recognized are:

- Mass balance and hourly capacity: some projects size all equipment on a higher than capacity mass balance (engineering companies may do so to ensure that the capacity guarantee is met – the customer pays the bill).
- Raw material and product mixes and specification.
- Design variables, such as environmental conditions maximum and minimum air temperatures, humidity, cooling water temperatures, catalyst aging, fouling, utility design pressures and temperatures.
- Unit operation and equipment design parameters.
- Uncertainty in physical properties and correlations.
- Safety factors.

As a standard approach we could say that:

A process engineer should cope with uncertainties where they really exist and avoid over-design on over-design.

An example could be the design of a heat exchanger. If there is uncertainty about the fouling factor, we either make a comparison in a similar application or take our best estimate, but we do not add an additional area for uncertainties in the calculation method. In general, these calculation correlations already have (as a standard) a probability of over 95% on the calculated result.

Timing/documentation: the over-design methodology needs to be documented in a report as part of the design basis to be prepared at the beginning of the conceptual design phase.

10.3.2.7 **Maintenance**

This is an often-overlooked activity at the design of a facility. It is however very important, as an objective of simple and robust designed plants is to opt for a maintenance-free plant. It will be clear that this is a target that we hope to approach, but even between the turn-around some maintenance might be necessary. Besides that, plants are subject to modifications during turn-around, so access is required for modification and maintenance.

The involvement of the maintenance function to a project is required for:

- Equipment selection, equipment monitoring, RAM specifications.
- Plot plan and lay-out development for accessibility of equipment that might be subject to maintenance or future modifications.
- Development of detailed lay-outs for small equipment, piping items and instruments for accessibility.

The contribution of the maintenance function should be based on a maintenance strategy for the plant under design. The strategy should cover the following elements:

- Predictive maintenance. This is focused on equipment monitoring, failure analysis based on historic data to predict upcoming failures, repair time predictions (particular important for the "*design for single reliable and robust components unless....*" design philosophy).
- Preventive maintenance. This is addressing timely replacement of equipment based on historic life cycle data.
- Breakdown maintenance. This is focused on the replacement of items after failure in a short time frame.

The maintenance strategy will have elements of different approaches, and must include repair times, round-the-clock service, spare parts, and contracting maintenance.

Timing/documentation: the maintenance strategy needs to be developed during basic engineering and used as reference for the project life from basic engineering up and to the operational phase.

10.3.2.8 **Construction**

The development of detailed construction plans, from the initial plan up and to the full-blown construction plan are essential for timely project delivery. The input from the construction function is required for:

- Plot plan and lay-out development.
- Major equipment dimensioning (field erection versus shop fabricated with reference to transportation).
- Project planning.

The construction plan must include the net work planning with, timing of deliveries, construction times, the sequence of installation of equipment, and critical pathways identified (C.I.I., 1986).

Timing/documentation: the preliminary and final construction plans are developed at different levels of detail over time. The first concept needs to be prepared during basic engineering, and completed during detailed engineering.

10.3.2.9 **Value engineering**

Traditional value engineering aims at eliminating or modifying items that do not add value for the company (Miller, 1989; SAVE International, 1997). Process simplification focuses on the elimination or combination of process units and/or equipment. Value engineering plays a role at equipment level. The same brainstorming group discussions are organized as discussed under process simplification, but the leading questions are focusing on a more detailed level.

Timing/documentation: as with the VIP process simplification, there are two levels of documentation. The team itself documents the brainstorming results, while the ideas developed and evaluated for implementation are reported by the project team. Timing is during the basic engineering stage.

10.3.2.10 **Implementation of VIPs in the work process**

The VIPs may be considered as:

- a separate item;
- a specific step in the work process; and/or
- a design procedure to be incorporated in a work process step.

Different companies make different choices regarding the types of VIPs and their implementation. The feasibility, conceptual design and basic engineering phases in a timeline are shown graphically in Figure 10.8. The points of application of the different VIPs are shown. It should be realized that the VIPs are also extending in the engineering and construction phases, and in the operational/evaluation phase. For instance, the VIP waste minimization but also maintenance and construction extend in these phases next to the evaluation of the all VIPs (Figure 10.9).

Evaluation of FEL and VIPs The evaluation of the project is an important point for the learning curve with regard to the work process and the quality of the design. The primary purpose of the evaluation is to check if the required objectives have been met.

The most important requirements are divided into process plant-related and project-related:

Process plant-related	*Project-related*
Capacity	Capital
Unit ratios	Timing
Flexibility	Start-up time
Product quality	

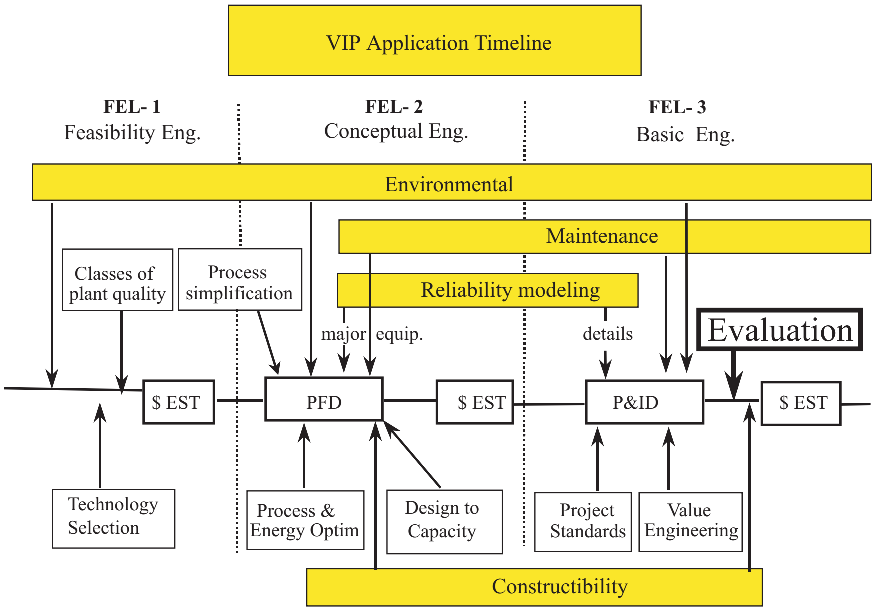


Fig. 10.8. VIPs implementation time line during FEL (Source IPA Inc.).

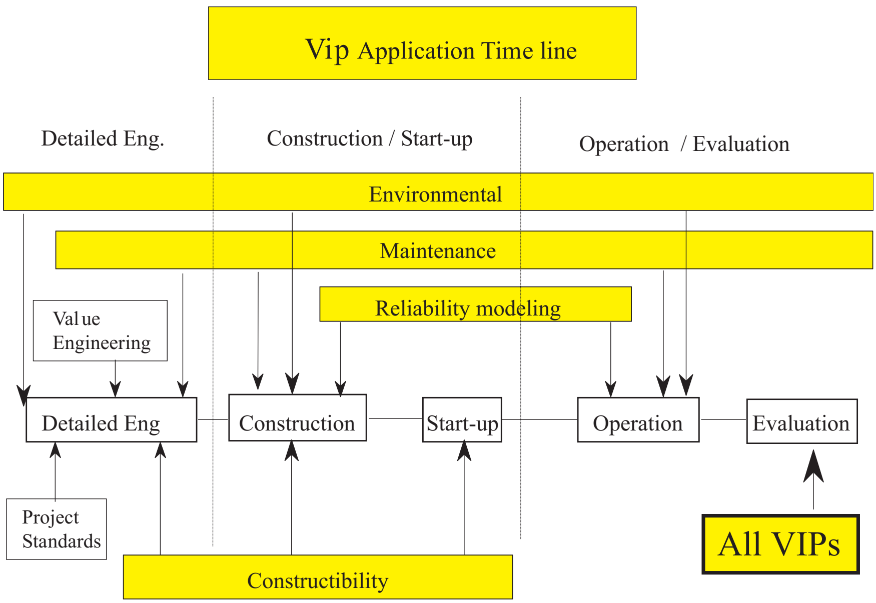


Fig. 10.9. VIPs implementation time line during: design engineering, construction and operation.

Timing/documentation: The evaluations will take place at two points in time: at the end of the FEL, to ensure the completeness and the quality of the design; and at the end of the project after start-up and the capacity run. A final evaluation report must be prepared for all involved disciplines.

Summary

The opportunities for the process industry are to improve the quality and efficiency of process plants and the design process

- The design process need to be based on a well developed work process, which is based on feed forward actions with limited feed back (reviews) adjustments and includes front end loading (a completed process design package) before detailed engineering starts. Such an approach allows concurrent engineering with considerable time and efficiency savings and with as target no rework.

The quality of the process plant is achieved by application of value improvement practices (VIPs) during the work process.

- The VIPs described shortly and considered crucial for a quality design are; technology selection, waste minimization, process simplification, process/ energy optimization, design to capacity, maintenance, value engineering and construction.
- The VIPs have to be applied during the design process, an overall time line was presented for implementation during design and engineering.

Appendix 10.1
Step Description of Preliminary Plot Plan and Lay-out (Example)

Description: The development of a preliminary plot plan and lay-out and a condensed form of the three- dimensional model with the major equipment and civil provisions. Provisions for future expansions supported by the business should be included.

Input:

Process information

- Index flowsheets, process flowsheets, equipment list, major equipment descriptions and dimensions, significant elevations.
- Logistic information as: (un)loading and storage requirements.
- Site and block drawings with neighbouring activities as; outside the fence activities, other plants, OSBL emergency and utility provisions, soil characteristics, loading facilities.

Safety information

- List of chemicals, quantities, their physical properties, safety hazards (toxicological data for people and environment, fire and explosion, inter-reactivity).

Output:

- Lay-out of the facility, two-dimensional drawings, and basic three-dimensional model.
- Major equipment location including structures, utility supplies as electrical transformers, supply headers.
- Lay-out of civil provisions.
- Roads, pipe bridges, control room, other civil work as draining, waste treatment.
- Lay-out of safety provisions.
- Emergency pond, fire-fighting system, emergency vent system.
- Area classifications.

Functions:	*Involved*	*Responsibility*
	Project/detailed engineering	Develops drawings and models with engineering disciplines input
	Process engineering	Provides process input
	Process control	Provides control input
	Manufacturing engineer	Operational input and requirements
	Logistic coordinator	Provides logistic requirements
	Environmental health and safety (EHS)	Environmental and safety requirements
	Maintenance and construction	Accessibility of facility

Procedures:

Company polices and procedures need to be followed.

The design should meet all local procedures either enforced by regulations or covered in covenants between authorities and the related industry.

Remarks:

Appendix 10.2

Function analysis During the arms race in the 1950s and 1960s, the U.S government wanted to review their military orders on cost. Therefore, initiatives were taken to evaluate the weapon systems, for what was called added value, through reviews and evaluations with brainstorming teams. This resulted in a discipline value engineering which is supported by SAVE International. This organization also sets up education facilities for professional value engineers. The U.S. government required the application of the value engineering technique for all their orders placed. The value engineering techniques were, during the last decade of the 20th century, also applied to process designs and equipment design by major companies, next to other application fields such as civil services. The value engineering technique is discussed below in its elementary form. For a full description, see the SAVE International Value Methodology Standard 1998

The technique is based on the evaluation of all kinds of systems with multi-disciplinary brainstorming teams lead by a value engineer (moderator experienced in value engineering). During brainstorming sessions, the objective is to generate alternative ways of achieving a certain function (target). The ideas generated are then evaluated on the added value versus the cost.

The value engineering process contains the following elements:

- Preparation as; set objective, collect information, select team, distribute information.
- Idea generation of multi-disciplinary team with functional analysis technique.
- First evaluation of ideas on applicability and value addition followed by a first screening.
- Second evaluation of ideas.
- Final selection and implementation of ideas.

The value engineering process is put into a time perspective in Figure 10.10.

At an early stage, is was recognized that the brainstorming sessions were not only crucial, but also that they were not always very effective, and differed in quality. It was Bytheway (1965) who introduced a concept – called “function analysis” – to facilitate the brainstorming part. The principal problem was that the team members had

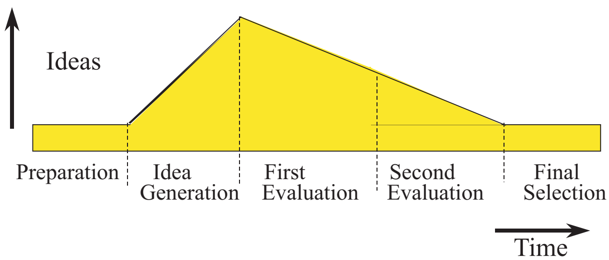


Fig. 10.10. Value engineering activities over time.

difficulty in finding the right abstraction level to generate out-of-the-box ideas. The concept of function analysis was later more extensively documented by Snodgrass and Kasi (1986), and nowadays it is embedded in a value engineering standard issued by SAVE International.

What is Function Analysis? Function analysis is a technique to determine what the functions are of different activities, leading to a certain product or state. The function is defined as a concise statement of what is being accomplished, without specifying how this is achieved. In a process plant, the overall function is to make from a raw material **A**, a quality product **B** to make a profit. The overall process is divided into different process steps (functions) to achieve the overall objective. The analysis of the functions is represented in a Functional Analysis System Technique (FAST) diagram, as shown in Figure 10.11.

Functions are described in only two verbs – an active verb, and a measurable noun. Examples of functions are:

- the function of a pump is, move material
- the function of a telephone is, facilitate communication
- the function of pencil is, facilitate communication
- the function of a distillation is, provide separation
- the function of a reactor is, convert chemicals

During the function analysis of a process plant, a process step diagram in sequential format from left to right is prepared. On the left side, we start with the raw material, and at the right we leave the diagram with product for the customer. The development of the FAST diagram is facilitated by the use of supporting words. Going from left to right, you can ask **HOW** to achieve the scope of the activities, while looking

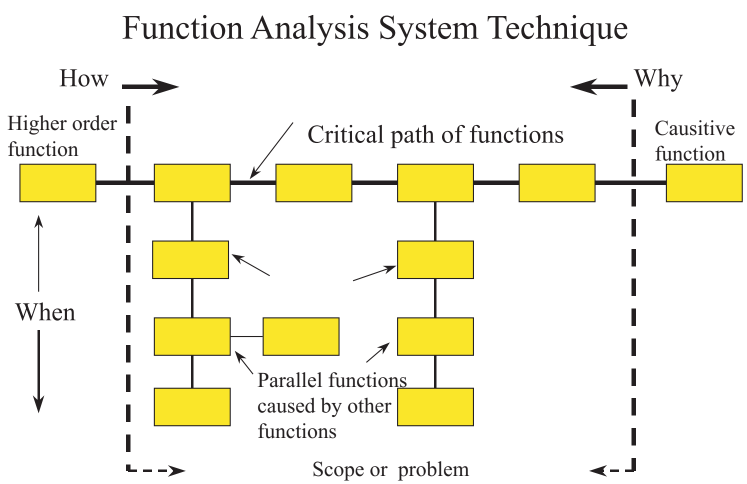


Fig. 10.11. Fast diagram.

from right to left, the question is **WHY.** On the vertical axes, **WHEN** questions have to be addressed to complete the fast diagram. A FAST diagram of a bakery is prepared and presented in Figure 10.12. The scope is to make quality pastries.

Brainstorming sessions based on function analysis are foreseen for the VIPs process simplification and value engineering. The alternatives created are evaluated based on cost, and added-value analysis.

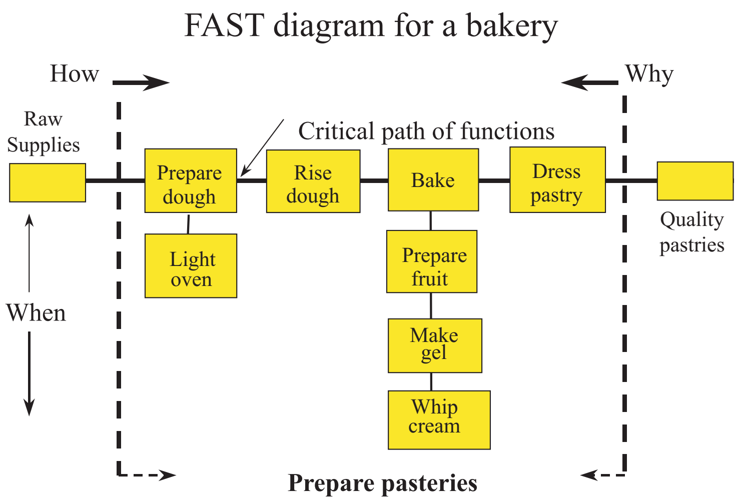


Fig. 10.12. Fast diagram of a bakery.

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Chapter 11
An Overview: Design of Simple and Robust Process Plants

11.1
Design Philosophies

An overview is prepared of what the design of simple and robust process plants includes. It summarizes the key elements, starting with a definition of a simple and robust process plant and followed by the 10 design philosophies. The list is continuous with the key elements in sequential order of the chapters. A simple and robust process plant can be defined as:

An optimal designed safe and reliable plant, operated hands-off at the most economical conditions.

11.2
Ten Design Philosophies to Achieve a Simple and Robust Process Plant

The ten design philosophies are as follows:

1. Minimize equipment, piping and instruments. The keywords for simplification and minimization of functions are: Avoid/Eliminate, Substitute, Combine/Integrate, Added value?
2. Design for single reliable and robust components, unless justified economically or safety wise.
3. Optimize design.
4. Clever process integration.
5. Minimize human intervention.
6. Operation optimization makes money.
7. Just-in-time production (JIP). With key elements: avoid or minimize logistic facilities.
8. Total quality control (TQC). With the key elements: prevent versus cure and first-pass prime production.
9. Inherently safer design. With the key elements: Minimize, Substitute, Moderate, Simplify.
10. Environmentally sound.

Design philosophies are an integrated set, and they must be seen as one set in order to achieve a simple and robust process plant.

11.3
Process Synthesis and Design Optimization

The design of simple and robust process plant demands adaptation of the design process to involve simplification, optimization and integration, with interaction between the different design activities:

Process synthesis methodology follows the adapted interactive onion model, which includes simplification and integration with iteration between the development steps (Figure 11.1).

Optimization for process design is a step-wise methodology within the process synthesis methodology, which must be applied to keep track of design decision. The methodology emphasizes step-wise reduction of the number of alternatives while increasing the number of design (sizing) variables, resulting in one selected and optimized design.

Clever process integration is applicable for utility as well as process streams; both streams require adequate back-up for control as well as operational reasons for independent operational processes or process sections.

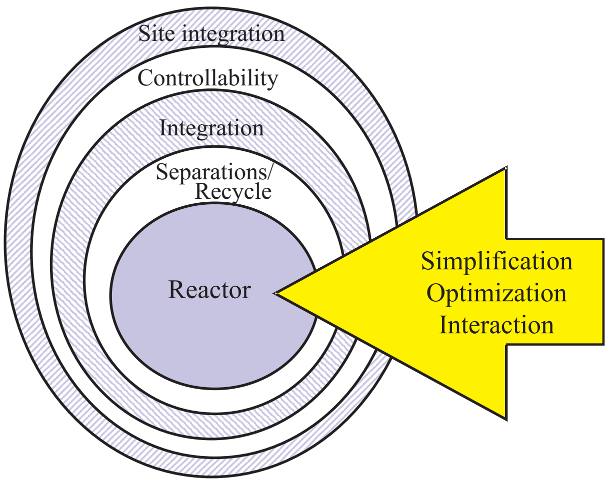

Fig. 11.1. The iterative onion model for process synthesis.

11.4 Process Simplification and Intensification

The technique for simplification and intensification cannot be generalized because each operation has its own solutions. However, it can be classified into categories to enable the thought process for development and application of simple designs. The simple design solutions for different units are ranked in sequential order of increasing complexity to support a designer in the design process.

11.4.1 Avoiding or Eliminating Functions

No storage – what you do not have cannot leak, and does not cost anything.

Transport of fluids can benefit from gravity forces and pressure differences.

Opportunities are process situations with repetitive actions called, do–undo–redo, like heating–cooling–re-heating, separation–mixing–separation, and pressurizing–depressurizing–pressurizing.

11.4.2 Combination of Functions

Reaction and reaction; Reaction and separation; Separation and separation.

Integration of equipment. Most equipment has the possibility to integrate adjacent equipment. This reduces not only equipment costs but also installation and piping costs.

11.4.3 Intensification of Functions

High surface area per volume, as for heat and mass exchangers.

Increase mass and heat transfer (kA and UA).

Benefit from centrifugal forces for phase separation, eventually combined with mass transfer or reaction, as in rotating packed beds.

11.4.4 Overall Process Simplification

Key elements are:

- Operation at 100% conversion.
- Adiabatic operations.
- Prevention of waste.
- Single train design and single component design.
- Selection of optimal pressure levels.
- Logistic strategy.

11.4.5
Ranking Order for Design of Simple Units

Apply ranking order of simplicity in units design, as for:

Reactors: liquid phase versus gas phase; homogeneous versus heterogeneous; adiabatic versus isothermal; tubular reactor versus CSTR.

Distillation: In increasing level of complexity for:

One- or two-component distillation; flash, stripper, absorber, dephlegmator, standard distillation.

Three-component distillation: one column configuration; side draw, divided wall column, side stripper, dephlegmator, two sequential columns.

Piping. Minimize the terms in the complexity function of piping

$$C = f\,(M)\,(N)\,(O)\,(Q),$$

where M is number of lines, N is number of valves, O is number of piping items, and Q is number of interconnections.

Instruments: Apply a defined instrument selection procedure based on the approach: “better a good reliable instrument then lots of unreliable ones”.

11.5
Process Design Based on Reliability

The design of simple and robust process plants is based on “single and reliable components unless...”. The quantitative bases to support this approach can be found in reliability engineering and reliability databases.
Reliability modeling is a mature technique to form a quantitative basis for process design.

Reliability studies are a tool to optimize the design of process plants based on the single-component philosophy. It has proven to be of high value, and now rational decisions can be taken around reliability and availability design issues.

Reliability availability and maintainability (RAM) specifications form a quantitative base for the purchase of equipment and supplies. Ram specifications require a partnership between supplier and receiver to obtain the maximum benefit.

11.6
Optimization of an Integrated Complex of Process Plants and Evaluation of its Vulnerability

Higher levels of process integration at a complex of process plants can bring considerable cost savings in logistic cost as well as operational cost. The logistic requirements for such a complex can be optimized based on reliability engineering techniques. The vulnerability of a complex can be quantified and design alternatives evaluated, to avoid over- or under- redundancy in designs, as a result of design policies.

Site selection has a very high and long-term impact on the operational cost. An objective site selection study is at least as important as technology selection.

Process selection within a product chain(s) and its level of process integration create a large benefit in logistic cost. Process integration can generate additional savings by integration of lower purity (less than commercial) intermediate product streams by avoiding/minimizing expensive separation steps.

Optimization of storage capacity for product chains must be based on reliability studies over the whole supply chain, including raw material and product transport system reliability.

Site vulnerability studies based on reliability calculations are to be performed for integrated complexes of process plants. Cost–benefit analysis can be performed of investments in logistic and utility or other back-up systems versus product availability to obtain a well-balanced, reliable, integrated site.

11.7 Instrumentation, Operation/Automation and Control

A simple and robust process plant is designed for total automation and hands-off control. This places extra emphasis on the design of instrumentation, automation and control.

Application of reliable and robust in-situ measurements with short response times is essential, as this is the basis for minimal instrumentation.

Total automation for hands-off operations puts specific requirements on the operational strategy, control strategy, safeguarding, and process observability.

The operational concept asks for development of an operational strategy to enable smooth start-up and shut-down, including interlocking with defined process states and transient pathways.

The concept of first-pass prime production (FPPP) requires preconditioning of all irreversible units, and the development of a detailed start-up procedure, in case of reactors based on dynamic rate models.

Alerting and alarming strategies are required which, next to its alarming function, in particular should address: alerting of operators to keep them involved, and the prevention of alarm showers to maintain an overview in an emergency situation.

Safeguarding of automated processes requires close observation of the critical process sections; this is effected by shadowing the operation with dynamic simulations. Deviation from normal operation can be detected at an early stage and used for timely process intervention. Critical process sections are, in particular, exothermal reactions and reactions with gas generation.

Observability demands specific measures for operation regarding process presentation, alerting, alarming, and control design.

Control design is a layered design consisting of: Basic process control layer (BPCL), including emergency control; Advanced control or model-based control layer; and Optimization layer. The basic control layer should function totally independently of higher layers.

Design of the basic control layer should be very robust. In case of failure of a higher layer, operation should still be able to run the process with minimal attention.

Robustness of basic control layer can be achieved by selection of the optimal pairing of CVs and MVs by application of static and dynamic interaction analysis. The selection of alternative CVs has to be evaluated for a self-optimizing control structure in case any interaction with the selected pairings is too large and would require a model-based controller..

The design of the model-based control layer should be based on a robust BPCL, and preferably designed on a first-principle dynamic simulation.

Model-based controllers are also designed as constraint controllers in order to maximize benefits from process capacity capabilities and fulfil quality requirements. These types of controllers are specifically important in combination with operation optimization.

11.8 Operation Optimization

The applications of operation optimization are growing. Specifically, off-line applications have found wide use in the field of production scheduling for batch-type operations as well as for continuous operations to determine static optimal operation conditions. Optimization of continuous process is based on first-principle models. Closed loop static optimizations, based on nonlinear programming techniques, for continuous processes are increasingly applied, but have still not reached their full potential. Dynamic optimization is applied initially to optimize transient operations.

The benefits of closed-loop static operation optimization are large in the order of percentages of the operational cost and capacity. The basic requirements are constraint controllers to push the process against its constraints, and robust and validated process models.

The methodology for closed-loop as well as open-loop process optimizations needs to be followed strictly to achieve a successful project. Too many projects have suffered from a recognized methodology not being followed.

The installation of a performance or profit meter is an important intermediate step for optimization. The meter gives valuable actual information on process operation in money terms. It is in use to compare actual performance with recommended performance from off-line optimization models. The performance meter is used as a stimulation for operation, to operate closer to its target (optimized) values. Another application is the validation of closed-loop optimization models which is quite important as any error in the model results in a lost opportunity.

The gap between the dynamics of the control of the process and the static closed-loop optimization, which normally runs on an hourly basis must be bridged. The self-optimizing control structure operating at basic control level was introduced.

This structure selects CVs for unit control to minimize the losses between two optimization cycles due to disturbances in balance with low level of interaction. In this way, complex multi-variable controllers can be avoided which are used to compensate for interactions of more conventional pairings of CVs and MVs.

11.9 The Efficient Design and Continuous Improvement of High-quality Process Plants

Continued improvement of existing plants are a requirement in order to remain competitive. Design projects for up-grading of or grass root process plants need to benefit from a working procedure to obtain a simple and robust process plant.

Continuous improvement of existing plants requires detailed observation and evaluation of: Process capacity performance; Process reliability and availability; Quality of operation; Optimal operation; and Opportunities for design improvements.

The design of high-quality plants requires the application of the iterative onion model for process synthesis.

Application of a detailed accepted work process that fits the organization.

Complete the front end loading (FEL) of a process design before detailed engineering begins, in order to manage a project within time, budget, and quality criteria.

Application of value improvement practices (VIP) to upgrade the quality of process design based on value addition criteria.

Functional analysis is a tool to facilitate an in-depth creative environment to generate and consolidate process simplification and value engineering opportunities.

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