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STUDIES ON COMPUTER AIDED PROCESS AND EQUIPMENT DESIGN IN PROCESS INDUSTRY

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Abstract

The challenge in design is to create a process or equipment for future needs. The changing world and keen competition bring about challenges such as a faster project time which means, on one hand, the need to utilize both earlier designs and organizational memory, on the other hand, that creativity should be supported to create competitive designs. At the same time requirements for a robust design in which uncertainties exist need to be taken into account.

The thesis presents new methods and application examples to answer the challenges. Case-based reasoning (CBR) provides a method for fast process and equipment design by utilizing earlier knowledge systematically. In new designs feedback from earlier experiences is taken into account, and a creative aspect can be included by the use of analogies. The thesis presents new method for CBR-based separation process synthesis and a CBR-based method for combinatorial mixer equipment design from parts.

A further challenge in design is how to create a robust and flexible design capable of operating in changing situations. The challenge has been dealt with scenario-based approaches and stochastic simulation. Three new applications are presented: Scenario-based approaches for thermo-mechanical pulp plant design in the presence of demand uncertainty and paper machine consistency control with an uncertainty in head box consistency control measurement. Stochastic simulation has been applied to paper machine broke tank level control, where the uncertainty is caused by paper machine breaks.

Tiivistelmä

Suunnittelun tarkoituksena on luoda prosessi tai laitteisto tulevaisuuden tarpeita varten. Muuttuva maailma ja kiristyvä kilpailu tuovat lisää haasteita suunnitteluun mm. tiukempien projektiaikataulujen muodossa. Tässä tilanteessa olemassa olevien suunnitelmien ja yritykseen kertyneen tietämyksen hyödyntäminen on tärkeää, kuitenkin samalla tavoitteena on tukea luovuutta, jotta kyetään luomaan uusia kilpailukykyisiä prosessiratkaisuja. Tämän lisäksi myös robustisuusvaatimukset on huomioitava, sillä tyypillisesti jo suunnitteluparametrit sisältävät epävarmuuksia.

Tässä työssä esitetään uusia menetelmiä ja sovellusesimerkkejä em. haasteisiin. Tapauspäättelyssä (CBR) olemassa olevia suunnitelmia hyödynnetään systemaattisesti uusien sovellusten luomiseen. Menetelmä mahdollistaa aikaisemmista suunnitelmista saadun palautteen hyödyntämisen. Tässä työssä esitetään uusi tapauspäättelyyn perustuva erotusprosessisynteesimenetelmä sekä tapauspäättelyä ja kombinatorista laskentaa hyödyntävä menetelmä sekoitinlaitteiston suunnitteluun saatavilla olevista osista.

Lisää haastetta suunnitteluun tuovat muuttuvien ja epävarmojen olosuhteiden aiheuttamat robustisuus- ja joustavuusvaatimukset. Tähän haasteeseen on vastattu skenaariopohjaisen lähestymistavan ja stokastisen simuloinnin avulla. Työssä esitetään kolme uutta sovellusta puunjalostusteollisuudesta: Skenaariopohjaiset lähestymistavat:

- termomekaanisen sellun (TMP) tuotantolaitoksen suunnitteluun, kun TMP:n kysyntää ei voida ennustaa varmasti
- paperikoneen sakeuden säätöstrategian valinta, kun perälaatikon sakeusmittauksessa mittausepävarmuus vaihtelee

ja stokastinen lähestymistapa:

- paperikoneen hylkysäiliön pinnankorkeuden säätöön, kun säiliöön syötettävän hylyn määrän epävarmuus johtuu paperikoneen katkoista.

Preface

The research included in this thesis was done at the Laboratory of Chemical Engineering and Plant Design in Helsinki University of Technology in 1998 to 2001 and in Oy Keskuslaboratorio KCL in 2002 to 2006. Financial support from Kemira Foundation, Research Foundation of Helsinki University of Technology, Foundation of SNIL ry. and the the Academy of Finland is gratefully acknowledged.

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List of publications

I Pajula, E., Seuranen, T., Koiranen, T., Hurme, M., Synthesis of separation processes by using case-based reasoning, *Comp. Chem. Eng.* **25** (2001) 775-782.

II Seuranen, T., Pajula, E., Hurme, M., Synthesis of azeotropic separation systems by case-based reasoning, *Computer-Aided Chemical Engineering,* Vol. 10, Elsevier 2002, 343-348.

III Pajula, E., Seuranen, T., Koiranen, T., Hurme, M., Selection of separation sequences by case-based reasoning, *Computer-Aided Chemical Engineering*, Vol. 9, Elsevier 2001, 469-474.

IV Seuranen T., Hurme M., Pajula E., Synthesis of separation processes by case-based reasoning, *Comp. Chem. Eng*. **29 (**2005) 1473-1482.

V Pajula, E., Koiranen, T., Seuranen, T., Hurme, M., Computer aided process equipment design from equipment parts, *Comp. Chem. Eng.* **23** (1999) Suppl. 683-686.

VI Sundqvist, S., Pajula, E., Ritala, R., Risk premium and robustness in design optimization of simplified TMP plant, *Computer-Aided Chemical Engineering*, Vol 14, Elsevier 2003, 311-316.

VII Pajula, E., Ritala, R., Measurement uncertainty in integrated control and process design – a case study, *Chemical Engineering and Processing* **45** (2006) 312-322.

VIII Pajula, E., Tienari, M., Studying broke tank averaging level control with stochastic simulator, *Proceedings of the Control Systems 2006 Conference*, ed. R. Ritala, Tampere University of Technology, Tampere 2006, pp. 43-48.

Author’s contribution

I The author developed the idea and participated in building the example applications and writing the paper.

II The author participated in developing the idea, building the example applications and writing the paper.

III The author developed the idea and participated in building the example applications and writing the paper.

IV The author mainly developed the first part of the methodology.

V The author participated in developing the idea, built the example application and participated in writing the paper.

VI The author participated in developing the idea, building the example and writing the paper.

VII The author participated in developing the idea, built the example application and participated in writing the paper.

VIII The author participated in developing the idea, building the example applications and writing the paper.

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Notation

a	proportionality factor for weighting the risk
B	tank level, %
b_{in}	flow to the broke tank, t/h
b_{out}	flow from the broke tank, t/h
c	broke tank consistency t/m^3, constant
$\overline{C}$	expected cost
$C_{capital}$	capital costs
$\overline{C}^S$	the expected cost of the stochastic model solution
C_W	worst case cost
C_W^R	worst case cost of the worst case analysis solution
D	percentage concentration of light key in distillate
f	the ratio of the molal flow rates of products (distillate and bottoms)
F	the control strategy depending on the tank level and control parameters
F	percentage concentration of heavy key in distillate
f_{in}	fiber flow to the process, t/h
$\mathrm{f_{out}}$	fiber flow from the process (paper), t/h
f_{trim}	trim broke, t/h
$g(n(t))$	operation costs of each scenario
m	number of years for depreciation
N	number of components in the separation problem, number of refiners
p^s	probability distribution of scenarios
p_{w}	scaling factor
$\mathrm{R(C^R)}$	purely robust model solution
$\mathrm{R(C^S)}$	stochastic model solution
V	volume of the broke tank, m^3

Greek

α	relative volatility
Δ	boiling-point difference between the two components to be separated
ε	tolerance value for worst case cost

η	scale parameter in Weibull distribution
μ	mean value
σ	shape parameter in Weibull and standard deviation in log normal distributions
σ^s	standard deviation of operation costs

Abbreviations

AI	artificial intelligence
BAT	best available technology
CBR	case-based reasoning
CES	coefficient for ease of separation
EHS	environment, health and safety
GA	genetic algorithm
MIDO	mixed integer dynamic optimization
MINLP	mixed integer non-linear programming
MSA	mass separating agent
THF	tetrahydrofuran
TMP	thermo-mechanical pulp
VLE	vapor-liquid equilibrium
XML	extensible markup language

1 Introduction

The purpose of engineering in general, including chemical engineering, is to create wealth and welfare. To accomplish this goal, the raw materials are transformed and/or separated into products. In process design new ideas to do this are created and translated into feasible process and equipment designs (Douglas 1988). Nowadays competition is keener and margins smaller (Barnicki and Siirola 2004), which means that there is a need for more sophisticated process synthesis, optimization and other design tools to aid in creating innovative new processes in less time. On the other hand the quality of design should be improved through organizational learning which can be accomplished by utilizing earlier experiences systematically. It is however more challenging than before to find the best alternative among feasible designs, because environmental, health, and safety aspects as well as requirements for product quality are more important than ever in getting the competitive edge. The challenges in process and equipment design are even more complex because at the early design stages the design problem is inherently ill-defined and external uncertainties, such as raw material availability or product demand, need to be considered too. During the design process the impact of uncertainties is minimized with different approaches: 1) rigorous modeling to include exact presentation of phenomena and physical properties, 2) process-oriented tools to include system effects and 3) knowledge-based tools to include earlier experiences and tacit knowledge.

The aim of this thesis is to find new or improved systematic approaches for the design tasks in presence of uncertainties. For conceptual process design case-based reasoning can be used for selecting separation operations and sequences by using creatively earlier knowledge as discussed in Papers I to IV. For equipment design case-based reasoning offers systematical approach for utilizing design cases, and since the design task is well defined, rigorous adaptation routines can be defined and carried out resulting feasible, automatically created designs (Paper V).

Uncertainties can be taken into account in design also by means of stochastic simulation or scenarios. This thesis examines the applicability of these approaches to pulp and paper industry design problems (Papers VI to VIII). The use of simulators has been emphasized since the computational effort is relatively large and suitable simulation tools are available.

2 Design stages

The typical process design stages, decision points and loops between the stages are presented in Figure 1 (adapted from Aittomäki et al. 2002). The aim of innovation stage is to generate ideas for creating new of improved processes which should be economic, safe and environmentally friendly. At the research stage the basic information for pre-feasibility study and process development on reaction chemistry, physical properties etc. is generated by literature survey and laboratory studies. After research phase first feasibility evaluation of the process is made.

Process development and pre-design take place closely connected and mostly parallel. Traditionally process development is mostly focused on experimental work in bench and pilot scales. Many of the experimental activities can nowadays be substituted by modeling and simulation. In fact conceptual design, which includes the development of process concept, combines process development and pre-design. The first preliminary process concepts are created already at the laboratory stage. They are further elaborated using bench and pilot experiments and simulations at process development stage and further at pre-engineering stage. The aim of pre-engineering is to create the real process concept for the plant and to make a feasibility study.

If the evaluation of the investment is accepted, the project continues with basic engineering, including sizing of process units, preliminary layout, etc. and detailed engineering including control engineering, mechanical design of the equipment, etc. After this the construction and start up stages remain.

The approaches presented in this thesis are related to the following steps of the process design stages, Figure 1: The CBR-based methods presented in Papers I to IV are applicable to the creation of process concepts in preliminary engineering and equipment designs in basic and detailed engineering (Paper V). However, the later design phases are of importance for instance in control system design. The approaches presented for dealing with uncertainties are applicable to cost estimation and sizing at the preliminary engineering stage (Paper VI), control system design in basic and detailed engineering (Papers VII and VIII) and tuning at startup (VIII).

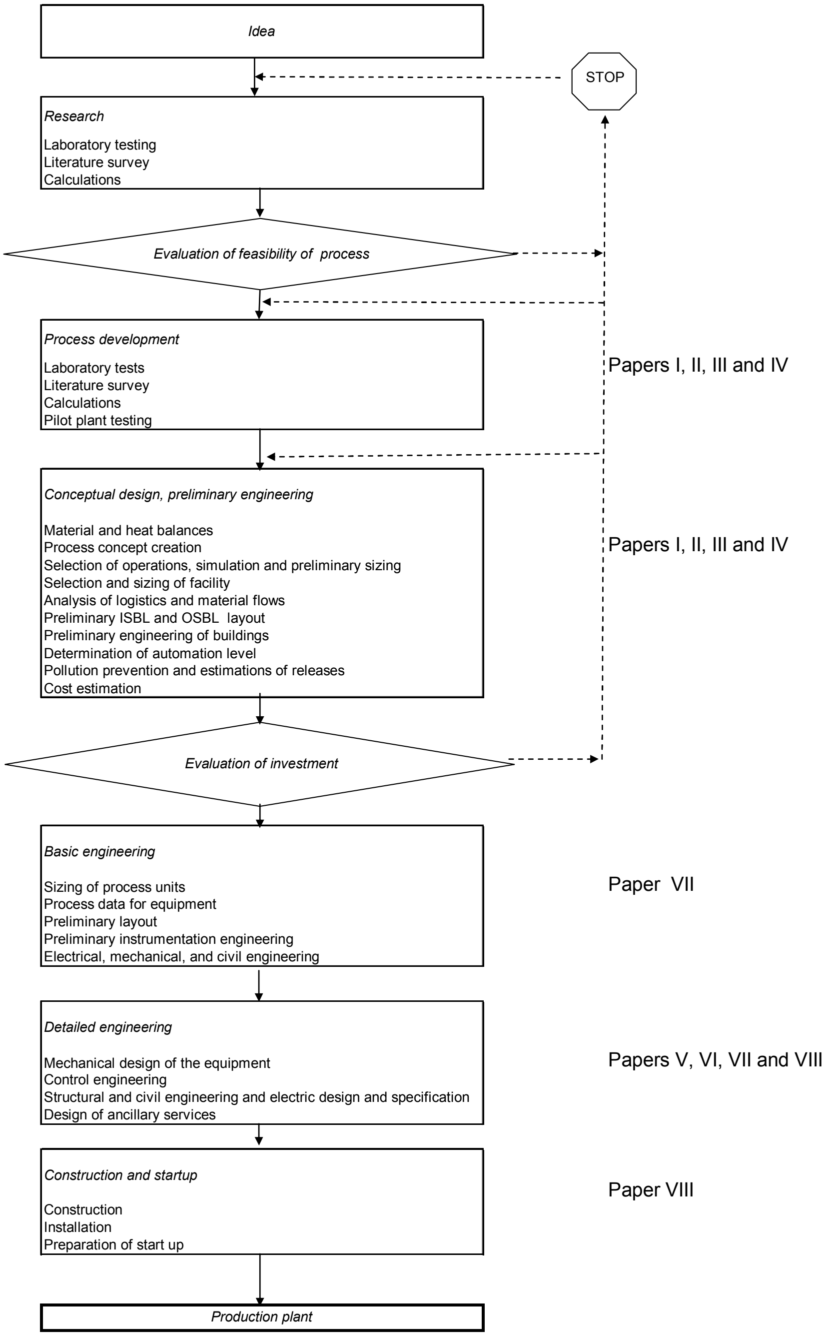


Figure 1. Process design stages (based on Aittomäki et al. 2002). Steps where the methods presented in Papers I to VIII can be applied are also pointed out.

3 Design challenges

At the early stages of process design, the outcome of an engineering project can be influenced the most. In a plant design project, 80% of costs are determined by preliminary design, even though only a minor part of the project time is used at this stage (McGuire and Jones 1989). The later the changes in design are made, the more expensive they are as seen in Table 1 (Bollinger et al. 1996). Therefore the challenge is to create the process concept with required properties as early as possible and avoid later conceptual changes because the cost and effect on project schedule are minor at the early stages compared to final design or construction.

Table 1. Relative cost of a process change at different design stages (Bollinger et al. 1996)

Process design stage	Relative cost
Research	1
Process flowsheet	10
Final design	100
Production	1000

More generally the challenges in design can be divided into:

1) Technical challenges, such as how to design flexible and clean plants, Chapter 3.2

2) Challenges in design process as discussed in the following:

3.1 Design process related challenges

Process design can be defined as a *creative* action to achieve the desired purpose, for instance a new product or profitable process to satisfy a particular need, taking into account constraints, such as physical laws, regulations and standards as well as time constraints (Sinnott et al. 2000). It is typical in design that on one hand creativity is needed to create new designs and improvements but, on the other hand, reliable existing design solutions should be utilized to ensure the maturity of the design. Therefore, the design methods should support both *creativity* and *the reuse of existing experience* which allows the corporate learning process. These aspects are combined in case-based reasoning (Papers I to V), which allows direct reuse of existing information with feedback on process performance. The CBR approach also supports creativity by allowing the use of analogies (Paper IV).

Engineering time is often one key issue in process design. A competitive edge may be achieved if the product is available at the market before the competitors respond to the changes in demand and markets. A shorter engineering time may be achieved with the use of simulation tools, design support systems, for example databases (McGuire and Jones 1989). In fact in case-based reasoning, time savings are readily available by using existing designs for creating new designs. By using the concurrent engineering approach, where the quality and external factors are taken into account at the early stages and design tasks are executed parallel to each other as far as possible, lead also to shorter project time. Savings up to 50% of design time have been reported with concurrent engineering (Banares-Alcantara 2000).

3.2 Technical challenges

Another challenge is that the process design tasks need to be performed in a constantly changing and uncertain environment. Therefore processes need to be *flexible and robust to disturbances.* Because uncertainty and variability parameters are inherent characteristics of all processes, methods for managing *uncertainties* are needed.

The uncertainties in process engineering can be classified as (Pistikopoulos 1995):

- Model-related uncertainties, describing the uncertainties related to the model; kinetic constants, physical properties, etc.
- Process-related uncertainties, describing the uncertainties related to the performance of the process itself; flowrate and temperature variations, stream quality fluctuations, etc.
- External uncertainties, describing the uncertainties from the environment; feed stream availability, product demands, etc.
- Discrete uncertainties for equipment availability and other random discrete events.

In the presence of uncertainties, the design objectives can be referred to as (Grossmann and Straub 1991):

- Design for fixed degree of flexibility (aim to achieve optimal design while ensuring feasible operation for any possible realization of the uncertain parameters)

Or

- Design with an optimal degree of feasibility (if trade-offs between flexibility and economics are explored) that determines the maximum deviation the design can tolerate while all continuous uncertain parameters are feasible

Approaches based on rigorous mathematical optimization exist for determining flexibility (Biegler 1997), but these mathematical models are time-consuming to create. Process robustness, ability to tolerate significant changes caused by the external environment, and flexibility requirements can also be approached with scenarios, for instance with the worst case cost as a measure of robustness in optimization (Paper VI).

It is well known that *control and process design interact* and they should be designed simultaneously. A process should work satisfactorily during transition from one operating condition to another as well as recover from disturbances. Mathematical programming-based approaches exist for simultaneous process and control design, for instance the rigorous approach by Mohideen et al. (1996) resulting in a large MINLP (mixed integer non-linear programming) problem. Another example of systematic approaches to the problem is the algorithm by Kookos and Perkins (2001) which analyzes a sequence of combined configurations and by the use of a bounding scheme reduces the search space. In the rigorous approaches, model correctness, reliability and applicability are essential, the models must have a wide enough range, and they need to be properly validated. For instance kinetic data and thermodynamic property methods are likely sources of errors if models are used outside the scope of their applicability (Klemola and Turunen 2001).

Different emphases in process synthesis leads to different process plant designs. Requirements for efficient energy and raw material usage lead to emphasizing process integration and intensification approaches, whereas EHS and sustainability requirements are the basis for inherent safety and clean technology viewpoints.

Process integration was defined in 1993 as a common term for the application of methodologies developed for system-oriented and integrated approaches to industrial process plant design for both new and retrofit applications (Gundersen 1997). One well-known example of process integration is the Pinch technology, where a heat exchanger network is designed to maximize process-to-process heat recovery and minimize the external utility loads.

Process intensification was defined at the 1970s as a “reduction in plant size by at least a factor 100” (BHR Group 2005). The design philosophy aims at radical reductions of the physical size of the process equipment, which means attempts to replace large, expensive and energy-intensive equipment with smaller ones, less expensive apparatus and possibly to combine some operations in smaller apparatus (Tsouris and Porcelli 2003). In some cases it is possible to produce better products and reduce capital costs. In addition, this approach provides several safety benefits (Etchells 2005).

The inherent safety approach aims at processes that are safe in their nature, not because of added-on safety systems. The inherent safety approach aims is at avoiding hazards, instead of controlling them. The inherent safety principles are:

- Intensification or minimization
- Substitution
- Attenuation or moderation
- Limitation of effects.

This approach usually leads to simpler and cheaper process plants, because the number of protective equipment needed is smaller, and smaller inventories are used (Kletz 1998).

Clean technology aims at reducing pollution. It is defined as “An installation that has been adapted to generate less or no pollution. In clean as opposed to end-of-pipe technology, the environmental equipment is integrated into the production process” (U.S. Environmental Protection Agency 2005). Therefore, clean technology is equivalent to inherent safety but in environmental aspects.

Conflicts exist within and between the process design approaches. For instance in inherently safe design, an intensified, smaller reactor may be considered safer due to a smaller amount of hazardous material in the reactor, but the reactor may require more severe conditions (temperature and pressure) or a more complex control system which has a negative effect on safety. The controllability of intensified or integrated processes may be a problem (Luyben and Hendershot 2004). Even though process robustness (i.e. ability to tolerate significant changes caused by the external environment) is also a strategy in inherently safer design, small holdup in inherently safer or intensified processes may lead to poor controllability. Some complications in the plant design may also be due to the flexibility requirements, which conflicts with the desire of simplicity in inherent safety (Kletz 1998).

4 Systematic approaches in process synthesis

Process synthesis is a creative action where the process flowsheet alternatives are created and evaluated. To be able to answer the multivariate and multicriteria challenges in process design, it is obvious that systematic approaches are needed. In this Chapter some trends in process synthesis are briefly described.

4.1 Heuristic approaches

Hierarchical approach to conceptual design (Douglas 1988) decomposes the design problem to a hierarchy of decisions, Table 2. The design procedure is executed to create a basic case design, and then the decisions and their impact on costs are analyzed.

Table 2. Hierarchy of decisions (Douglas 1988)

Level 1.	Batch versus continuous
Level 2.	Input-output structure of the flowsheet
Level 3.	Recycle structure of the flowsheet
Level 4.	General structure of the separation system
	a. Vapor recovery system
	b. Liquid recovery system
Level 5.	Energy integration

Another example of hierarchical approaches is the onion model (Smith 1995). This approach starts with reactor system design (type and conditions), then the reactor and separation system. Finally the heat exchanger network and the utility systems are designed (Figure 2). In this approach many decisions can also be evaluated only after completing the design, even if the hierarchy tries to minimize the interactions between the steps, presented in Table 3.

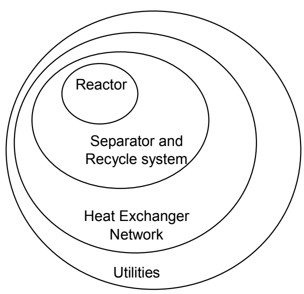


Figure 2. Onion model (Smith 1995)

Table 3. Process synthesis steps in the onion model (Smith 1995)

Step	Action, comments
1	Choice of reactor, raw material conversion very important
2	Choice of separation, e.g. distillation, phase separation, absorption
3	Synthesis of reaction-separation systems, recycling needs to be considered
4	Distillation sequencing, usually no need to study simultaneously sequencing and heat integration
5	Heat exchanger network and utilities targets
6	Economic tradeoffs, taking into account reactor conversion, inerts, need for heat exchanger network
7	Effluent treatment, waste minimization
8	Process changes for improved heat integration
9	Heat exchanger network design, e.g. pinch technology

In the sequential hierarchical approaches, external factors (for instance site selection, solvent availability, emission permits, etc.) are considered only when they cannot be neglected anymore, which often causes many iteration loops and rework. Parallel hierarchical approach (concurrent engineering) takes the external factors into account from the beginning, and different design tasks are executed parallel to each other. If some uncertainties exist, the designer will use a few alternative designs. It is not unusual to achieve 30% savings in development costs and 50% in time (Banares-Alcantara 2000).

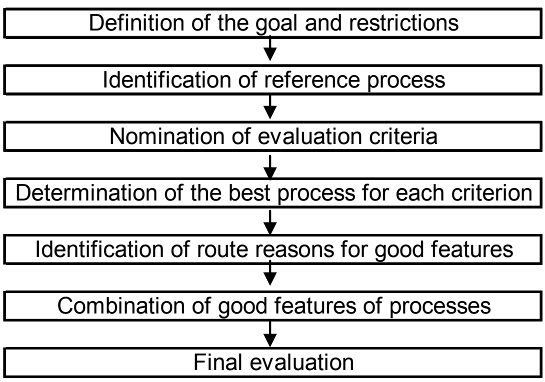


Figure 3. Evaluative approach for process development (Cziner et al. 2005)

Cziner et al. (2005) have presented an evaluative approach which is based on analogous processes. The processes are studied and compared with design task at hand. The best processes according to different criteria are determined, and root reasons for the good features are identified. The good features are combined, which often leads to conflicting aspects and principles. The recognition of conflicts helps to concentrate on key problems, and innovative modifications in processes are required. The steps of the method are shown in Figure 3.

4.2 Phenomena- and conflict-based approaches

Lately two new approaches have been developed based on identifying process phenomena and conflicts in design objectives. In phenomena-based methodology for process intensification (Rong et al. 2004) process phenomena (for instance the oxidation reaction) are identified and manipulated for the generation of improved designs. The methodology consists of three steps: first the process is analyzed and all relevant phenomena are identified, secondly the phenomena are analyzed and manipulated based on process intensification principles and finally applied in practice to generate new intensified process alternatives.

Conflicting process objectives can also be taken into account in process synthesis by systematical analysis. In the conflict-based analysis (Li et al. 2003), derived from the TRIZ methodology, the design system is modified by overcoming its internal contradictions. This conflict-based approach has potential for gaining more efficient solution in the subsequent MINLP stage.

4.3 Optimization-based methods

Optimization-based methods are called *mathematical programming*. A mathematical programming problem (typically mixed integer nonlinear programming, MINLP) consists of objective function and equality and inequality constraints. In the problem both continuous and discrete variables exist, which complicates the optimization procedure. The continuous variables can for instance describe the states (temperature, pressure, etc.) or flow rates. The discrete variables describe the topology of a process network or represent the existence or non-existence of unit operation. Nowadays more and more complex optimization problems can be solved as the theory and implementations develop further (Sahinides and Tawarmalani 2000), but at the early stages of process design not all the variables needed for the superstructure to be optimized are known. Building the superstructure is also time-consuming. *Mixed integer* *dynamic optimization* (MIDO) problems differ from MINLP problems by including dynamic models in the problem description. Mathematically this means differential algebraic equations. Dynamic models are needed for instance when comparing controller performances and tuning them.

Genetic algorithms (GA) can be applied in the process synthesis, for instance distillation sequencing design (Hurme 1996). The multicriteria (cost, safety and environment) aspect can be achieved using an analytical hierarchy process in the cost function (Cziner and Hurme 2003).

The basic steps of the genetic algorithm are the following:

1. The generation of an initial population. The size of the population depends on the complexity of the problem.
2. An objective function (for instance analytical hierarchy process or sum of individual column vapor flows) is used for the evaluation of individuals.
3. The generation of a new population with a crossover procedure.
4. The mutation of sequences at a randomly chosen location. Both the separation method and sequence is mutated.
5. The selection of the best solutions and the deletion of the worst ones.
6. The repetition of steps 2 to 4 until the solution does not improve within a given tolerance.

4.4 Phenomena-driven approach

According to (Pohjola et al. 1994, Tanskanen et al. 1995) "(Chemical) process is control of (physico-chemical) phenomena for purpose." It can be presented as an object that has attributes: Purpose, Structure, State and Performance (PSSP). This set of attributes is necessary and sufficient to describe the properties of any real thing. The approach is based on selecting the needed phenomenon, for instance reaction, instead of unit operation in process. The PSSP methodology is also applicable to the design activity itself.

4.5 Knowledge-based approaches

In the last decades, more rigorous calculation methods have become available for chemical engineers. However, in spite of their possibilities, the current approaches are not able to describe reliably every physical phenomenon and engineering practice. Neither it is always reasonable nor possible to make all the rigorous time consuming calculations at the early stages of design for all process alternatives. In practice, engineers use their experience and general knowledge first to select, which alternatives are reasonable for further studies and thereafter proceed with more advanced methods, for instance rigorous simulations. To systematize and support these activities knowledge based approaches can be used.

Knowledge based methods consist of symbolic and non-symbolic computational methods. The symbolic methods are usually based on symbol manipulation and logic. Many non-symbolic methods can be classified as soft computing: methods which imitate nature (fuzzy reasoning, neural nets and genetic algorithms). One approach to non-symbolic manipulation is to use search methods. In this approach the solution to the problem is searched by trial and error. In this method the problem is the combinatorial explosion. One way to limit possible alternatives is the use of heuristic knowledge. When heuristics are unavailable, genetic algorithms that imitate nature's evolution can for instance be used. Logic is an important part of artificial intelligence (AI), but it tells nothing about the efficiency of utilizing the information available. The knowledge available is often inaccurate, unclear or insufficient. In these cases conventional logic fails and other approaches are needed. Useful ways to deal with the problem are fuzzy logic and case-based reasoning (Hyvönen et al. 1993).

Several AI applications have been created for process design and equipment selection. For review see Stephanopoulos and Han (1996). Only very few of these use systematically existing proven knowledge instead of rules.

5 Separation process synthesis

At the early stage of process design, conceptual design, the basis for further design activities is created. The conceptual design stage for a new commercial process costs usually 10 to 20% of the total development cost, but these decisions account for 80% of the total project costs (Douglas 1988). At the conceptual design stage, experience has shown that less than 1% of the ideas are successful, so quick screening of different process alternatives is needed (Stephanopoulos and Han 1996). If only a few alternatives exist, considering all possible separation combinations may be feasible, but because the combinatorial explosion takes place quickly when the numbers of products to be separated increase, systematic approaches are needed. In this section a few ways to design a separation process are briefly described.

5.1 Rule-based approaches and heuristics

A way of designing a process is applying heuristic rules. For instance Nath and Motard (1981) have created an approach where an initial separation process structure is created by simple heuristic rules like ”favor the smallest product set”, “favor distillation”, etc. After that every rule is challenged and alternative process structures are created.

Based on these heuristics it is sometimes difficult to define which separation to do first. This problem has been approached by defining equations that make the alternatives comparable. For instance Nagdir and Liu (1983) have introduced a set of seven ordered heuristic rules, 1) favor ordinary distillation and remove mass separating agent first, 2) avoid vacuum distillation and refrigeration, etc. These rules are simple to apply and don’t require a mathematical background or computer skills. Nagdir and Liu also proposed an equation for the coefficient of ease of separation (CES) for distillation. CES takes into account the relative volatilities or boiling point differences of the components to be separated and the ratio of molar flow rates of distillate and bottoms, Equation 1.

$$CES = f \times \Delta \qquad (1)$$

where f = the ratio of the molal flow rates of products (distillate and bottoms)

Δ = boiling-point difference between the two components to be separated

Another approach is the ROTE equation for distillation (Porter and Momoh 1991). It is calculated from relative volatilities, mole fractions in the feed, and the ratio of minimum reflux and reflux ratio. The basic assumption is that the optimum sequence is the one that requires the smallest binary distillation total vapor load.

Barnicki and Fair (1990, 1992) have created a very large rule-based system for reducing the number of process alternatives in a separation process synthesis. Unlike previously mentioned systems, they also consider gas/vapor mixtures and a larger number of possible separation processes as favored separation methods.

5.2 Residue curve maps

Distillation is the most mature separation method in fluid separations (Barnicki and Fair 1990) but still new designs are found. For instance, an interesting approach in distillation process design is to use the information included in residue curves, see for instance Fien and Liu (1994) and Wahnschafft et al. (1992). King et al. (1999) have applied residue curves to select separation sequences for ternary azeotropic separations. Petlyuk (2004) has lately also published a book on distillation theory and design based on residue curve maps.

5.3 Design based on physical properties

The relation between physical properties and separation techniques can also be the basis for a separation process synthesis. Jaksland et al. (1995) applied the idea that an optimal separation process flowsheet also satisfies the feasibility limits for the proposed separation method. They calculated several relative properties, for instance melting and boiling point ratios, and compared these values with predefined feasibility limits. This method is applied in the created CBR approach (Paper III) for finding out feasible retrieval parameters. The feasibility limits for each separation method are presented as trapezoidal numbers (Qian and Lien 1995). The order of separations is defined by weighted relative ratio values, the biggest one presents the easiest separation and it is carried out first.

5.4 Hierarchical approach

The hierarchical method of Douglas (1988) has been extended to a separation system synthesis (Douglas 1995). The method utilizes the rule-based approaches (for instance Barnicki and Fair 1990, 1992).

5.5 Fuzzy algorithms

Qian and Lien (1994) applied a fuzzy match inference strategy in a separation process synthesis. In their approach, continuous variables and qualitative information are described as fuzzy sets. A proposed solution and heuristic rules are compared and fuzzy matches calculated. The feasibility of a solution is the better when the solution matches better with the rules. Qian and Lien (1995) also presented the idea of using trapezoidal numbers for presenting rules.

5.6 Genetic algorithms

Genetic algorithms (GA) (see also 4.3) can be used in a process synthesis. Hurme (1996) applied a genetic algorithm to a five-component separation problem with ordinary and extractive distillation as a possible separation method. He found out that the approach was fast compared to random optimization and not as computationally intensive as mathematical programming methods. Fraga and Senos Matias (1996) have applied genetic algorithms for optimising a preselected sequence of distillation units for a three-component azeotropic separation. The GA method was extended by the Analytic Hierarchy Process, which allowed both economic and sustainability aspects to be included in the synthesis (Cziner and Hurme 2003). Later consideration of uncertainty aspects was also included by adding a stochastic simulation level (Cziner et al. 2006).

5.7 Mathematical programming

Mathematical programming has been successfully applied to a separation process synthesis, for instance the optimisation of non-ideal and azeotropic distillation processes (Bauer and Stichlmair 1996). With mathematical programming approaches, the optimality of the result depends on the accuracy of the mathematical model. For example Bansal et al. (2002) have applied the parametric programming method to a new, multicomponent, mixed-integer dynamic distillation model with uncertain parameters including also control parameters. The problem is highly combinatorial by nature, with over 1900 discrete design alternatives. Nevertheless, the MIDO (mixed integer dynamic optimization) algorithm presented in the paper converged in just five iterations.

5.8 Shortcut-based comparison of separation methods

Shortcut-based comparisons are used in many approaches for selecting separation methods. The selection task is challenging, because most approaches lack generality and are difficult to update as the technology develops. Shortcut methods are often used to deal with the problem, but they are not very accurate or applicable to all alternatives, although simple to apply. For instance Souders (1964) has compared separation factors (α's) required in distillation, extractive distillation and extraction. Null (1980) compared the energy use of melt crystallization and adsorption to distillation and developed comparison curves for the purpose. For VLE-based separations, Jobson et al. (1996) have defined capacity variables that make distillation and other VLE separation processes, for example equilibrium flashes in series or parallel, economically comparable.

The process synthesis does not end when a certain method is selected. For example in distillation, heuristic rules may be appropriate when considering further ideas and process alternatives, for instance thermally coupled distillation flowsheets (Rong et al. 2000b). Another example of complex new approaches is the hybrid membrane/distillation process, in which there are several flowsheet alternatives to consider (Pressly and Ng 1998).

6 Case-based reasoning

Case-based reasoning (CBR) is one of the non-symbolic AI methods. It imitates the human thinking trying to find a solution based on earlier experiences and adapt a proven solution to a current problem. The method uses systematically the most similar existing problems and their solutions to create a solution to a current problem (Kolodner 1993). If there are plenty of existing solutions available and adaptation is based on well-known physical phenomena, feasible solutions can be found even without rigorous calculations.

Case-based reasoning differs from other major artificial intelligence approaches by utilizing specific knowledge of earlier experienced situations (cases) instead of relying only on general knowledge or generalized rules between problems and their solutions (Aamodt and Plaza 1994). A typical CBR system consists of four parts: retrieval, reusing, revising and retaining (Figure 4). The current problem is defined as a query by giving the essential parameters for instance feed components, their physical properties and product purity requirements in case of a separation problem. Based on these, the similarity is calculated and a user-defined number of the most similar cases are retrieved. The user can select a case and launch an adaptation routine, for instance a scale-up calculation. General knowledge is often also used in the adaptation.

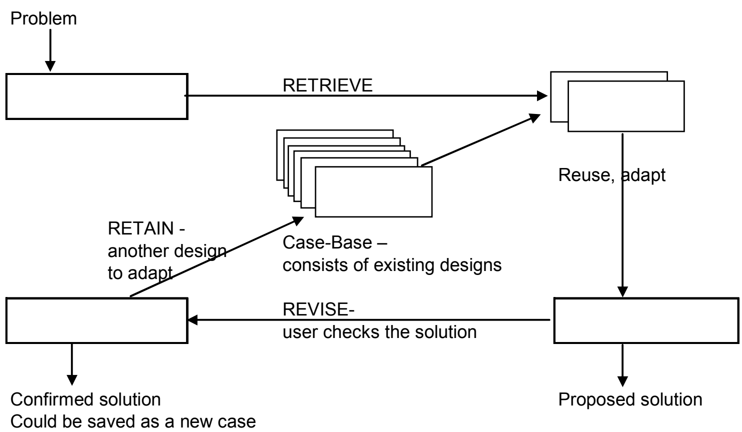


Figure 4. CBR cycle (modified from Watson and Marir 1994)

6.1 Applicability

CBR is beneficial when the problems are not completely understood so that an exact model cannot be built, and for example experimental work and/or earlier experience is required. The problem does not need to be completely defined before starting to reason possible solutions. Failed experiences should also be included in the case base, because they warn about possible failures. As an approach, CBR proposes solutions quickly and in this way fastens and directs the design process. On the other hand, the old cases should not be used blindly. Sometimes it may also be difficult to find the most appropriate set of cases when reasoning (Kolodner 1983a, 1983b, Cunningham 1998). The quality and maturity of cases and adapted designs is discussed further in Chapter 7.3.

6.2 Tools

Several commercial tools for creating CBR systems are available, for instance ReCall and CBR-Works as discussed by Seuranen (2000). These tools provide the ability to develop applications easily and quickly, but they also limit the flexibility in case representation, learning and adaptation (Aamodt and Plaza 1994, Seuranen 2000). Of the eight readily available commercial tools studied by Seuranen (2000), none were considered flexible enough for chemical engineering purposes. For instance CBR-Works only supports 1 to 1 relation and relational databases, which limits the usability of the object-oriented approach. For instance in the mixer selection application presented in Paper V, Visual Basic together with Microsoft Excel was used because of limited possibilities for adaptation routines in commercial CBR tools. In the heat exchanger design application (Seuranen et al. 2001), object oriented programming was used in creating the basis for more time-consuming rigorous simulation studies. In this application CBR made it possible to take experience-based knowledge (fouling, feasible heat exchanger types) into account at the early design stages. CBR-Works 4.0 was utilized when creating the queries in process synthesis demonstrations (Papers I and III). Different general tools can be utilized in building CBR applications. For instance lately Rizal and Suzuki (2005) have applied new XML (extensible markup language) technology in building a CBR-based abnormal condition management system.

6.3 Applications to design

CBR applications can be found in several fields of design, for instance in process and equipment design (discussed later), structural design in civil engineering, architectural design as well as meal planning (Maher and de Silva 1996). Many of these contain little or no adaptation. This is understandable because adaptation may be difficult and when applying adaptation rules the advantages of the CBR approach such as no generalizations and results based on proven cases, are diminished. Cunningham (1998) also points out that for now the most successful CBR applications contain no or very little adaptation. A review on case-based reasoning in design is presented by Maher and de Silva (1997).

6.4 CBR in process engineering

Even though CBR applications have been applied to several application areas, only few of them appear in process engineering. Some examples are described below.

6.4.1 Process design

Surma and Braunschweig (1996) studied case retrieval and similarity in process engineering and created a successful demonstration for retrieving the most similar process flowsheets for hydrogenation C3 process. They calculated the similarity of cases, i.e. flowsheets, as graphs. First the class of flowsheets was selected from the case base, and then the similarity between the flowsheet objects was calculated to limit the number of cases to those that fulfill the necessary requirements. Thereafter the structural similarity was calculated. The most similar graph is the one that has the largest similar sub-graph with the current query. Another approach is the transformation distance approach; i.e. the most similar graph is the one that has the smallest least-cost set of transformation operations to transform it to the current problem. This retrieval approach seems to work well with rather simple flowsheets. Once relevant cases have been retrieved, the design can benefit from the system by browsing through the found cases and selecting the most applicable ones for the current design. For adaptation and more complex processes more background knowledge is needed. These areas were not considered in the paper.

King et al. (1999) studied ternary azeotropic separations by using residue curve maps (RCMs). The cases stored in the case base included physical data on components, azeotropes, distillation boundaries and regions. The approach is presented in more detail in Chapter 8.

Arcos (2001) has presented a CBR application T-Air for designing chemical absorption plants. The similarity between cases is defined by chemical knowledge. The case representation consists of input knowledge including the customer-given specifications for instance washing liquid, chemical case-model, flowsheet and annotation that give the reasons for the current decisions. The case retrieval is made in two stages, first cases are retrieved based on relaxed input data and then refined with domain criteria and interactions with the user. Usually, the new problem is solved using parts of solutions in different cases. In the adaptation phase, a precise model and all the equipment parameters are defined. This application decreased the time for analyzing solutions.

Avramenko et al. (2004) have applied CBR in a decision support system for waste water treatment. The system includes three databases (equipment, flowsheets and methods), a CBR module and a conceptual design builder module, the last of which is used when CBR fails to find an appropriate solution. In the definition of similarity, the features, their relations and their numerical values are taken into account.

Heikkilä et al. (1998) and Hurme and Heikkilä (1999) have applied CBR for safety evaluation. CBR was used to evaluate the value of one subindex in an index-based approach for the evaluation of inherent safety. Using process characteristics as retrieval parameters, the nearest cases, where accidents or minor incidents have happened, were found from the database of good and bad designs. The found cases were scored to a Safe Process Structure Subindex. In this way their safety features are available for process synthesis by a genetic algorithm.

Seuranen et al. (2001) presented how inherently safer process alternatives can be applied to new designs based on a CBR with existing inherently safer cases and accident cases.

An example of CBR combined with other AI methods is a hybrid blackboard-based expert system and case-based reasoner used in the design of an injection-moulding process (Kwong and Smith 1998). Usually the number of trial runs needed for determining moulding parameters depends on the experience of the personnel. This kind of heuristic knowledge and experience cannot be utilized well in an expert system. Also, available mathematical models were not good enough. In the hybrid approach, a blackboard-based expert system is used for generating the process solution and CBR system for quickly setting the moulding parameters based on earlier experiences. The CBR system has simplified and fastened the parameter determination.

6.4.2 Equipment design

CBR has been applied for instance to mixing equipment selection and design (Kraslawski et al. 1995). An interesting feature in the mixing equipment application is that rather rigorous adaptation routines are included in the application. In this thesis the mixer equipment design was extended to take into account commercially available equipment parts (Paper V). The application is discussed in more detail in Chapter 8. Other applications have been created for shell-and-tube heat exchangers (Koiranen and Hurme 1997, Seuranen et al. 2001), and solid-liquid separations (Virkki-Hatakka et al. 1997). In the heat exchanger application an input file is created with the CBR system for a commercial simulator package for further studies.

Lately CBR has been utilized in a decision support system for pre-selecting column internals in reactive distillation (Avramenko et al. 2005). In vibrofluidized bed selection (Kraslawski and Kudra 2001), fuzzy and rough set adaptation routines have been created. In the rough set approach, innovative design is enabled by fixing the parameter value range 20% broader than in the retrieved cases. The adapted output parameters differ completely between these approaches when the input parameters in retrieved cases are very similar and output parameters different between cases. In these cases the membership function approach in fuzzy adaptation fails, whereas the rough set adaptation gives good quality results.

Woon et al. (2005) have been able to speed up conventional design methods in pneumatic conveyor systems design by utilizing CBR. The CBR approach helped decrease the amount of simulations needed in defining air velocity, bend type and bend angle to obtain a good particle size distribution as output.

6.4.3 *Control and fault diagnostics*

CBR has also been applied to the process control (Roda et al. 1999) of a biological wastewater treatment plant. In this process the inflow and the population of the micro organisms vary, the amount of detailed knowledge of the process is limited and only a few online analyzers are available. Weather conditions also affect the process. The CBR system informs the operators about the successful control strategy of the most alike situation in the past. This system cannot deal with conditions that have not occurred in the past, but it makes quick solutions possible when similar cases are found in the case base.

One of the fields where several applications can be found is fault diagnosis. For example a CBR system has been developed for fault diagnosis and decision-making in pulp processes (Xia et al. 1997). The system integrated with information management systems and distributed computer systems gives possibilities for quick solutions when a problem occurs and the process is not dependent on operators' experience alone.

6.5 Comparison of CBR and other process synthesis methods

CBR was selected to be studied because no other methodology brings systematically all existing knowledge available and therefore is able to create a basis for innovative environment. Since the knowledge is stored as cases, also tacit knowledge related to existing designs is more efficiently stored than in model- or rule-based methods. Comparison of process synthesis approaches is presented in Table 4, and the methods are discussed in more detail in Chapter 4. Still today there exists no systematic method for separation process synthesis that also fulfills the practical requirements (Cziner et al. 2005).

Table 4. Comparison of process synthesis methods (Cziner et al. 2005)

	MINLP	GA	CBR
superstructure required	yes	yes	no
combinatorial explosion	very much	much	some
non-interactive method	yes	yes	no

7 CBR in separation process synthesis

Papers I to IV present a new methodology for selecting separation methods based on earlier solved design cases and the knowledge stored in them. If the solutions are of high quality and there are several options that resemble the current problem, most of the information needed is included in the existing designs. This utilization of existing data can be done systematically by CBR.

Earlier only King et al. (1999) have applied CBR in the design of separation systems. They studied only ternary azeotropic separations but by using residue curve maps (RCMs). The cases stored in the case base included physical data on components, azeotropes, distillation boundaries and regions. Based on the description, the system was able to generate several alternative azeotropic separation systems consisting of three columns. The similarity of the cases was based on the number and type of azeotropes (binary or ternary, minimum, maximum or intermediate boiling) based on RCMs, process objectives and performance indexes based on component purity and distillation regions as well as a qualitative description of the process; process units are described in terms of their relative position within the RCM.

The hypothesis in the CBR process design synthesis study is that CBR can be utilized in process synthesis provided that the available database is extensive enough. As the database consists of cases the maturity of which is defined, it potentially gives feedback on uncertainties in different alternatives. The engineering knowledge related to distillation and other separation methods can be extended by using the CBR approach in process synthesis. Even though distillation is very mature separation method, tacit knowledge related to distillation process flow sheets and other practical design aspects are important in design. These aspects are however not included in the rigorous distillation sequence synthesis methods such as optimization based approaches (MINLP, GA).

7.1 Method for CBR based separation process synthesis

The approach to separation process synthesis procedure described in Paper IV consists of the selection of 1) single separation methods, 2) separation sequences and 3) hybrid separations. This synthesis approach also takes into account the more complex alternatives in distillation sequencing and the possibilities for combining operations. The steps in this approach are:

1A *Selection of single separations*

a) search for the feasibility of conventional distillation-based operations
b) search for azeotropes
c) search for suitable mass separation agent (MSA)
d) search for other separation methods
  i) calculation of relative physical properties
  ii) search for separations based on the relative physical properties

1B *Selection of azeotropic separations*

a) search for separation in columns, isobaric conditions
b) columns, non-isobaric conditions
c) separation by using MSA
d) separation by using MSA and non-isobaric conditions
e) separation by other means; reactive, membrane, extraction, etc.

2 *Separation sequencing by using search criteria*

- component names or types
- relative volatilities
- VF values (Equation 2)
- coefficient of ease of separation (CES) values (Equation 1) of components (Liu et al. 1983)

and applying

a) sequences in found cases
b) sequencing heuristics (if stored in the cases)

3 *Search for combined operations*

The sequence synthesis is based on the calculation of VF criteria (Paper IV)

$$VF = \left(D + \frac{1.1F}{\alpha - 1} \right) N \qquad (2)$$

where

D = percentage concentration of light key in distillate

F= percentage concentration of heavy key in distillate

N= number of components in the separation problem

α= relative volatility

These steps are discussed in more detail in the following chapter.

7.1.1 Selection of conventional distillation separations

In the presented method single separations are selected first. Paper I presents a CBR-based methodology for this purpose. The similarity is defined by comparing different characteristics between the user input and existing design cases in the database, for instance phases present, process mode, the type of components to be separated or the shape of vapor-liquid equilibrium curve, feed and distillate concentrations, etc. The primary targets of cases, for instance removal of a solvent as waste or purity requirement for the waste water, can be used when calculating similarity as discussed in Paper I, which also gives examples.

7.1.2 Selection of single azeotropic separation

If azeotropes are present, the separation task is more complicated. Papers I, II and IV present that the selection of azeotropic separation can be done by using case-based reasoning. The *separation concept is defined by product and feed concentrations, azeotrope composition and the mixture solubility (i.e. is there a phase split).* If these criteria are analogous to the found case, especially relative to the azeotropic point, the process concept can be reused.

For instance the parameters used for searching the separation method for a pyridine water solution to be separated into products containing 1 and 40 wt-% of pyridine are azeotropic compositions (94°C and 57 wt-% pyridine), solubility with water (total), feed and product compositions. In the nearest found cases, the azeotropes were not crossed either, and distillation in a single column without an entrainer was proposed (Paper IV).

In more complicated cases the synthesis of azeotropic separations can also be made by *using several CBR searches* (Paper II). The searches are made in the following predefined order to find the most common and proven approaches first:

1) Separation in single column in atmospheric or non-atmospheric pressure
2) Separation in multiple columns in non-isobaric pressure

3) Separation by using MSA
4) Separation by using MSA and non-isobaric pressure
5) Separation by other means; reactive, membrane, extraction
6) Separation by hybrid separations

For instance, when the separation methods for a dilute (1wt-%) pyridine water solution are studied, suitable retrieval parameters are selected first. The separation is not simple because pyridine and water form an azeotrope. The separation method has to cross the azeotropic composition and purify the feed to the desired product compositions of 99 and 1 wt-% pyridine. Using these features as retrieval parameters, a suggestion of a tetrahydrofuran (THF) separation system is found; see Figure 6 in Paper I. A similar two-column separation strategy can also be applied to pyridine separation in a similar azeotropic crossing situation with a similar type of entrainer. The question whether a similar entrainer can be found is not answered by this CBR search, but it can be checked manually from the VLLE property handbook or by searching as summarized in the next chapter. In fact cyclohexane and benzene are found to be analogous solvents for pyridine based on the principles discussed in the next chapter. Therefore the separation concept can be directly applied.

7.1.3 Selection of mass separation agents

To compare other separation methods with mass separation agent-aided operations, or to replace an existing MSA with a more suitable one, a suitable MSA is needed for each separation, which cannot be made by conventional distillation in a feasible way. The first CBR search can be made by using component types and names as retrieval parameters, as described in Paper III. Their similarity is defined with a taxonomy tree (Figure 6). The taxonomy tree is based on the idea that components belonging to the same class have most similar properties, the deeper in the tree structure their closest common node is, the bigger similarity value they have.

A more accurate search can be defined by using concentrations and relative solubility parameter, polarity and dielectric constant as retrieval parameters (Paper II).

Paper III presents a case on finding a MSA for separating a 50 wt-% component from water to a 90 wt-% product. Ordinary distillation is not applicable since there is an azeotrope at 71 wt-%. The first search is made by using component types and presence of MSA as retrieval parameters. A more detailed search is made using also additional retrieval parameters: solubility parameter, dielectric constant and dipole moment. The two closest cases found propose several possible MSA's. This is a realistic result, since at least diisobutane, cyclohexane and diisopropyl ether have been reported for this separation in literature. Papers II and III give further example on MSA selection and replacement.

7.1.4 Other separation methods

It is often important to consider also other separation methods than ordinary distillation as discussed in Paper III. Therefore it is necessary to consider all the possible properties that may be utilized in separation processes and make a search based on these. The principle is to apply the separation method that utilizes largest property difference of the components to be separated. To do this relative properties are calculated for component pairs and compared to predefined feasibility limits (Jaksland et al. 1995). For example crystallization is considered very feasible, if the relative melting point ration is greater or equal to 1.2, and feasible if it has a value between 1.1 and 1.2. The approach is used for finding the most important retrieval parameters for CBR, i.e. the parameters that show greatest potential for separation of the species that have too small α's for ordinary distillation. In this way the amount of retrieval parameters is limited to essential ones.

7.1.5 Separation sequences

In CBR based separation process synthesis the separation sequence can be defined either by applying the heuristics description stored in the nearest cases (e.g. textual description in Paper III) or concluding the sequence based on the separation sequences stored in cases (Paper IV).

In the latter approach the suitable retrieval parameters can be component names or types, relative volatilities, CES values (Eq. 1) describing the ease of separation (Paper III) or VF values (Eq. 2) indicating the separation difficulty (Paper IV).

7.1.6 Combined operations

Papers I and IV discuss a combined operations separation sequence synthesis. The idea is that after the separation sequence synthesis, the user should consider combined

separations operations. This can be done by combining separation operations and studying their feasibility one by one. This kind of separation process units may also be included in the cases. They can be found from the case base with different approaches:
1) Combine two sequential separations. Then search if analogous combined separation can be found from the database using for instance relative volatilities, or
2) Calculate VF search criteria. Search combined separation cases for those VF values.

Searching for possible combinations may lead to fewer columns in hydrocarbon separation processes, when non-condensable gases are taken out of a condenser as a third stream (Paper IV).

7.1.7 Application example

It is characteristic to process development that many conceptual routes are considered at the early stage and reduced down to a small number for further investigation. It is coming increasingly important to be able to screen quickly large number of process alternatives as the time to market and on the other hand development cost need to be reduced. Therefore there is a great need for this kind of screening tool (Cordiner 2001). In the following an example of feasible separation sequence selection is given (Paper III). The example is complex as also other methods than distillation is needed for the separation task. The task is to separate a mixture of ethyl benzene (20 wt-%), m-xylene (40 wt-%), o-xylene (20 wt-%), and p-xylene (20 wt-%).

Step 1): Searching with α's and reactivities. It is concluded that ethyl benzene can be separated by ordinary distillation. The heuristics in the found close cases in the database are:

1. Perform difficult separation last and favor a 50/50 split.
2. Perform difficult separation last and use CES for finding the distillation order.

The heuristics no. 2 was selected. According to CES first o-xylene and then ethyl benzene are separated by distillation. For m/p-xylene separation the available relative volatility is too small.

Step 2): To separate m-xylene and p-xylene, an MSA is searched. No feasible MSA was found for case where both components are aromatic and have low polarity.

Step 3): To find a suitable separation method for m/p-xylenes, reasonable retrieval parameters are needed. This means that the relative parameters need to be large enough to make the separation possible. The possible calculated parameters are a relative melting point and relative kinetic diameter ratios. The parameters and calculated relative properties are presented in Paper III, Table 4.

Step 4): The database was searched using these relative parameters and including only cases in which at least one separation was classified as "difficult" based on relative volatilities. Two possible methods were found for m/p-xylene separation: molecule sieve adsorption and crystallization (Table 5 in Paper III).

Step 5): The separation sequence is concluded from found heuristics: first separate o-xylene, then ethyl benzene by ordinary distillation, and the separate the mixture of m- and p-xylenes by molecular sieve adsorption or crystallization.

The case study shows that CBR approach combined with heuristics is applicable to complex synthesis tasks where other separation methods than distillation are needed. The resulting separation trains are feasible and discussed earlier for instance by Morbidelli et al. (1986).

7.2 CBR implementation used

The hierarchical structure of case base is based on classification of separations as described in Paper I. Each process document contains general data for each separation existing in a separation train. Since every separation process consists of several separation steps, lot of step specific information is needed to be stored too. Link between the process description and equipment specification is created using relational attributes. In the example applications presented papers I to IV first draft implementation was made using MS Excel and larger application using commercial tool CBR-Works 4.0.

Every separation process consists of several pieces of process equipment, which have to be selected. The tree structures and some relational attributes have been presented in Figure 3 in Paper I. In separation process synthesis no practical and general adaptation rules exist due to the complexity of the synthesis task. However, some shortcut methods exist for different separation methods, for instance for adapting distillation conditions as discussed in Paper I. In our process synthesis case studies adaptation was based on human interaction and the combined operations approach, Chapter 7.1.6. Another possible, but too time consuming approach, was building the system from scratch ourselves using for instance XML (extensible markup language) technology.

7.3 Structure of case base and similarity

An advantage in the CBR approach is that the user can focus the search and divide the problem to sub-problems by defining different retrieval parameters for different separation tasks. The presented approach can also contain general rules, which can be described as general cases as presented in Figure 5. The general cases, as rules, cover a large area of process characteristics, but the degree of detail is much smaller than in proven cases. It is important that negative cases, i.e. failures, are also stored in the case base, because they help preventing the earlier mistakes.

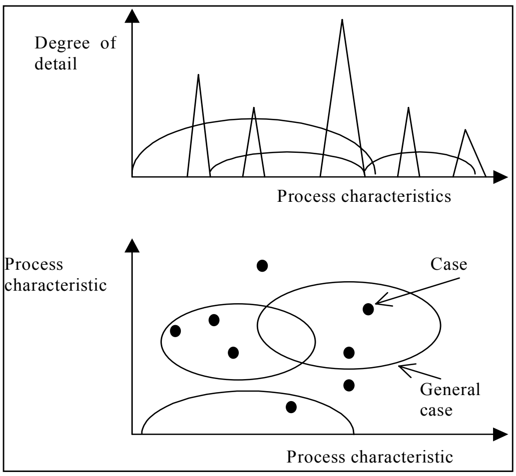


Figure 5. Structure of the case-base with detailed and general cases (Paper I)

The quality of the solution found and applied to the current problem depends on the quality of the solutions stored in the database and the validity of the adaptation rules included in the process. The quality of the solutions in the case base depends on the technical maturity and the performance of the proposed solution. Both aspects need to be considered in order to distinguish technically mature, well-proven strategies from promising but less mature methods, which may lead to an even better result. The quality of the cases is therefore described in Paper I by two factors, technical maturity and technical performance, which are described in Table 5. As new research or application results are published, the most applicable method may change, which requires that the database needs to be simple to update.

Table 5. Technical maturity and performance factor (Paper I)

Factor values	Description of technical maturity	Description of technical performance
0		Failure/ unsafe
1	Process idea or concept exists	Out of date
2	Process with basic engineering package exists	Modest efficiency
3	Plant in demonstration scale exists	Average efficiency
4	Operating plant exists	Proven good efficiency
5	Process is in wide use	Best available technology (BAT)

Similarity can be described in a tree-like structure, i.e. for instance the closer the component types are in the tree, the bigger similarity value this characteristic has, see Figure 6 (Paper I). Another approach can be the use of distance functions, i.e. the smaller the difference the values have within a predefined interval the bigger the similarity they have (Eq. 3.). For instance the similarities between solvent concentrations a and b (%) can be calculated in this way.

$$Similarity = 1 - \frac{|a-b|}{100} \tag{3}$$

A detailed review on the similarity concept in CBR is given by Avramenko and Kraslawski (2006).

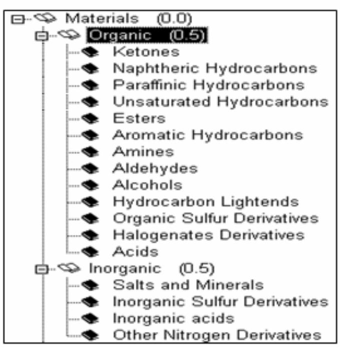


Figure 6. A part of the taxonomy tree for material types (Paper I).

7.4 Creativity and organizational learning aspects

Paper IV presents ideas on how to support creativity and organizational learning. The system should not only be capable of modifying old designs included in the database but also capable of creating new designs. One possible way of including creativity into the synthesis is to use analogies. Analogies can be included by using generalizations and other structural features, such as proper hierarchy. The introduced generalizations may include general level categories in the database, such as type of separation, type of components or their physical properties.

The idea of using cases also allows conflicting designs and failures to be stored systematically and no rigorous model structure is needed for storing the data. Storing failures as negative cases is important so as to prevent making the same mistakes again, and storing conflicting cases provides ideas for creative process designs. CBR systems also provide learning mechanisms and possibilities for feedback when the case base is maintained systematically. The CBR approach provides a flexible way of storing data and may also be used as a company's institutional memory, as proposed in Paper I.

7.5 The applicability of the synthesis method

The thesis presents a new approach to separation process selection and sequencing for azeotropic and non-azeotropic distillations but also other separation methods (Papers I to IV). The proposed CBR based separation process synthesis method is applicable especially in conceptual process design for screening options for further more rigorous studies by simulation. The advantage of this approach compared to rule-based approaches is that the knowledge is stored in detailed cases and can be utilized in a non-reduced form. The method is flexible because the knowledge can be searched using different retrieval parameters and weighting factors depending on the user's viewpoint. Also missing data can be handled easily in this approach by more general cases (i.e. rules). Vague criteria such as safety or operability, that are difficult to quantify, can also be included in the case base more easily than into an optimization cost function.

It is the characteristic of CBR that it depends on the existing data stored in case base. The information in database is to be extended and updated all the time based on the data extracted from the literature and new design cases done. Therefore the case base can form an institutional memory of the company. The design quality can be improved through the reuse of experience from existing designs. Therefore the feedback and practical experience gained from the previous designs should also be stored in the case base. This also improves the documentation practice in the company.

The benefit of CBR also depends on the engineering skills of the designer using the tool. The information in case base can be reused in an interactive and flexible way to solve different types of problems starting from routine problems, where the aim is to fasten and automate the design work, to problems requiring creativity, where analogies are employed. The benefit of CBR approach compared to modeling is that tacit knowledge (know-how) in existing design cases can be more extensively reused through the interactive employment of CBR case base.

The main limitation of the approach is the database, which needs to be extensive enough to cover the area at hand, because only minor adaptation can typically be carried out especially in process design, due to its complexity. The database is however all the time extended as discussed before.

Results from Papers I-IV have been compared with literature data. The conclusion is that the CBR approach is applicable to the separation process synthesis tasks and the resulting designs agree with the cases reported in the literature. The proposed method can however be considered mainly as a preliminary idea generation and screening tool in process design and the separation sequences generated need to be studied further more rigorously by simulation.

8 CBR in equipment design and selection

In equipment design the size of the system to be designed is often smaller than in process flowsheet design. Therefore fewer variables are needed to give enough information to make a feasible equipment design or selection in comparison with process synthesis. Adaptation rules can also be more easily defined explicitly, and it is often possible to conclude, which design parameters can be defined based on the experiences stored in case base. Earlier research on this area has been discussed in Chapter 6.4.2.

8.1 Proposed method

Unlike the separation process synthesis problem in the previous section a design process of one piece of process equipment is often a well known and more precisely defined problem, in which similar calculations are repeated. Therefore, rigorous adaptation rules can be created for example for a mixer equipment design (Paper V).

Paper V presents a new approach to equipment selection from feasible combinations based on lists of parts. The system presented in Paper V differs from the earlier application created by Kraslawski et al. (1995) in the more detailed selection of mixer equipment. A new feature in the approach of Paper V is the use of combinatorial calculations in creating feasible mixer parts combinations. This approach is an excellent basis for more rigorous studies when the system does not behave ideally. It cuts also down the amount of experiments needed.

The application developed in Paper V includes the basic parts of the CBR applications presented in Chapter 6 such as normal database functions, such as the storing of cases. Existing design cases consist of process and design parameters and lists of equipment parts. The mixers are often made by assembling from parts, which can be combined in several ways. To automate the selection of a feasible combination all possible combinations are created first at the program development stage. This is done beforehand, because even though several rules are applied to limit the combinations to feasible ones, the combinatorial explosion occurs very fast. Therefore, the time-consuming combinatorial calculations need to be carried out only if the lists of parts are updated. The basic steps of the system usage are:

1. The user defines the mixer problem
2. The five nearest cases are retrieved, and the user defines which case to adapt
3. The mixing tank dimensions are adapted based on the selected case or defined by the user
4. The criteria for suitable mixers is defined based on the data given by the user and found in the nearest case
5. The suitable mixers are selected from the feasible combinations and reported to the user.

Some of the decisions can be made based on the nearest case found, for instance the average bulk velocity and number of impellers can be selected based on the nearest case. The data of the described problem and design data from the retrieved case can be used also as inputs for design equations e.g. for adaptation. The user defines the mixing problem by giving a fluid volume, average bulk velocity in the tank, fluid viscosity and density and possibly tank dimensions. There are usually several cases similar enough for adaptation in this case, therefore, the five nearest cases are presented to the user and the user selects which one to use for adaptation.

In the application in Paper V, the adapted design is presented as a specification sheet, and a list of alternative designs is created based on the specified properties, such as the similar impeller type, maximum power greater than the power required.

9 Coping with uncertainties in process design

Nowadays it is usually possible to solve a problem using computational models, provided that the problem can be precisely formulated and all (physical and chemical) phenomena can be described as a model accurately enough. Data and programs needed for problem-solving can also be stored as the storage capacity of computers has increased. It is, however, not enough to predict the system performance at a single point but robustness issues also have to be studied. Robustness refers to the system's ability to perform well even under unusual conditions. Typical ways to evaluate robustness are worst case cost, which may be too conservative, and with probability distributions. Still, the computational effort for analyzing large uncertainties may be too high in comparison with the assurance gained, and in some cases the use of a few scenarios and a weighted cost function may be a better approach (Sargent 2005).

Even if rigorous process models can be created, they are never perfect. Very often the models lack some phenomena or simplify them. For instance measurement uncertainty has very seldom been included in rigorous process studies, even though it may even be the decisive factor in control structure selection as presented in Paper VII.

The motivation to make some uncertainty related studies with scenario-based and stochastic simulation was to test these well-known approaches with simplified process models related to pulp and paper industry to see whether these approaches would give relevant information on the effect of uncertainties. It was also considered to go further in mathematical optimization feasibility and flexibility studies. These methods however require rigorous modeling as well as plenty of exact parameters, which make them often too complex and time-consuming to build and simulate in process design projects. Therefore, in this study the emphasis was put on scenario-based and stochastic approaches.

9.1 Scenario-based approaches

Even though mixed integer dynamic optimization systems have been proposed, for instance Bansal et al. (2002), providing a framework for optimizing design problems involving dynamic phenomena, defining an accurate process model to be optimized still remains a difficult task, and uncertainties involved make it even more complicated. This problem can be approached with scenarios. Scenarios can be defined as possible sets of events in the future (Anon. 2005). A major additional difficulty in integrated process and control design is that as the dynamic behavior is optimized, the specifications must state the dynamic scenarios under which the process will be operated and the relative frequency of occurrence of these scenarios. Such information is not readily available from business considerations guiding the project, and only rarely from control or process engineers, but from the strategic analysis of the company's operating environment. As the scenario data will strongly affect the design, robustness against uncertainty in scenarios should be verified.

Dynamic simulation has been applied earlier in pulp and paper industry to grade change dynamics (Lappalainen et al. 2003) and disturbance diagnostics for agitated pulp stock chests (Ein-Mozaffari et al. 2003), for instance. Optimization has also been applied to paper trim loss minimization (Harjunkoski et al. 1996), for example. However, so far there have been very few publications that take into account uncertainty in realistic design optimization problems. In the process design case study presented in Paper VI, the uncertainty in product demand is taken into account with scenarios, and the results have been further studied with a risk premium approach and using worst case cost as a robustness measure. To the authors' knowledge, both risk premium and robust optimization using worst case cost as robustness measure have been applied to thermo-mechanical pulping for the first time in Paper VI.

In Paper VII the effect of measurement uncertainty is studied with disturbance scenarios in a simplified paper machine short circulation case study. It is shown that measurement uncertainty may be the decisive factor and should not be neglected in integrated process and control design. To the authors' knowledge, this kind of study concerning the effect of paper machine head box consistency measurement accuracy on the optimal controller alternative has not been published earlier.

Risk premium can be understood as the reward for holding the risky market portfolio rather than the risk-free asset (Anon. 2005). The idea of the risk premium approach is to weight both the expected cost and the risk of optimization problem. The measure of risk can for instance be standard deviation of operation costs of different production scenarios, σ^s, as presented in Paper VI.

The objective function, total cost to be minimized can be expressed as

$$C_{tot} = \sum_{1}^{S} p^S g(n(t)) + C_{capital} + a\sigma^S . \qquad (4)$$

where

$g(n(t))$	operation costs of each scenario
p^s	probability distribution of scenarios
$C_{capital}$	capital costs
a	proportionality factor for weighting the risk
σ^s	standard deviation of operation costs.

Robustness describes the parameter insensitivity of stability to changes in the system. The robust optimization study (Paper VI) can be based on e.g. the worst case scenario analysis (Suh and Lee 2001), for example. The best robust solution is chosen amongst the Pareto optimal design alternatives, when the expected cost the (optimal solution of the stochastic model) and robustness measure (worst case cost) are simultaneously optimized. The robust model is based on the stochastic model having an additional objective of controlling the variability of the performances of individual scenarios. The worst case scenario is taken as the objective variable for the robustness measure and a decision-making procedure is introduced to choose the best robust design alternative for the case study.

In the robust optimization procedure, the expected cost and the worst case cost are simultaneously optimized by the ε-constraint method (Miettinen 1999), so that the value of the worst case cost is restricted to the tolerance interval

$$\varepsilon = [R(C^R)\ R(C^S)] \qquad (5)$$

where $R(C^R)$ is a purely robust model solution (minimum of the worst case scenario)
$R(C^S)$ is the stochastic model solution (worst case value of the stochastic model minimum point).

The best robust solution for decision-making can be found for example by using an L^2 *metric* method (Suh and Lee 2001), i.e. by minimizing the function

$$f = (\overline{C} - \overline{C}^S)^2 + \left[p_w(C_W - C_W^R)\right]^2 \tag{6}$$

where $\overline{C}$ = expected cost

$\overline{C}^S$ = the expected cost of the stochastic model solution

C_W = worst case cost

C_W^R = worst case cost of the worst case analysis solution

p_w = scaling factor

9.1.1 Demand uncertainty

An optimal design of a thermo mechanical pulp (TMP) plant (Paper VI) is based on the pulp demand of a paper machine. The design parameters to be optimized include a number of refiners (N_{Ref}) and an optimal storage tank volume (V_{tank}) of the plant. The optimization is a dynamic problem with the paper machine demand, number of active refiners and utility costs varying in time. In the TMP plant design, the optimum of the total costs is found via a subtask of minimizing the utility costs in operations and scheduling optimization.

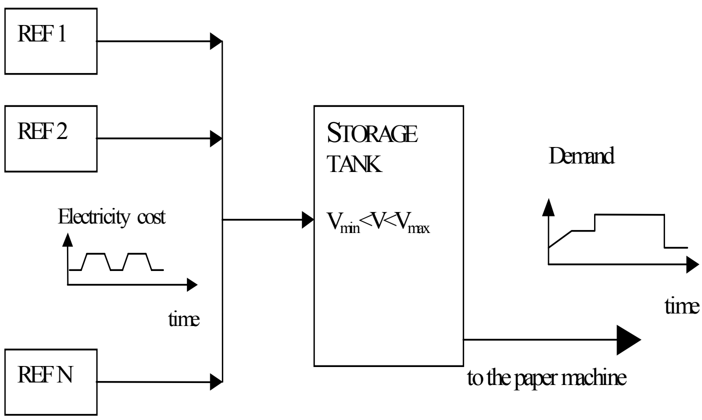


Figure 7. Simplified TMP case

The design of a simplified TMP plant (Figure 7) was optimized with a risk premium using four different demand scenarios of the paper machine (Figure 1 in Paper VI). In the multiobjective design problem the worst case scenario (representing the highest cost) was taken as a robustness measure and the design parameters were determined as a trade-off between the optimalities of a stochastic model (expected value of all scenarios) and the worst case scenario.

TMP design optimization is a MINLP problem, since it has both a discrete (N_{Ref}) and a continuous (V_{tank}) design parameter. The operational optimization subproblem includes integer variables (number of active refiners in time) as well as process dynamics (the demand of a paper mill, electricity cost) having inequality constraints of minimum and maximum tank volumes. Even though the case was over-simplified, an effective solution algorithm was required for the optimization of a two-day production period introducing 100 time intervals. A simulated annealing algorithm (Otten and van Ginneken 1989) in a Matlab environment was found to be effective in obtaining optimal operational values for the number of active refiners at each discrete decision time. By adding the capital costs, the optimal values for decision-making amongst various discrete design alternatives (N_{Ref}, V_{tank}) were obtained.

Design with a risk premium. The expected value based on the probabilities of all scenarios was calculated for each discrete design parameter (N_{Ref}, V_{tank}). The risk premium was taken into account as the standard deviation of the different scenarios with a proportionality factor $a = 0 \ldots 3$.

In the case, the risk premium affects the design only for an intermediate number of depreciation years, Figure 8. It was obvious that the number of years for depreciation (corresponding to the relative capital costs *versus* operational costs) had a strong impact on the option for the best design alternative. With 10 years depreciation time for capital costs, the risk premium factor had an influence on the optimal design increasing both the number of refiners (N_{Ref}) and the continuous design parameter (V_{tank}).

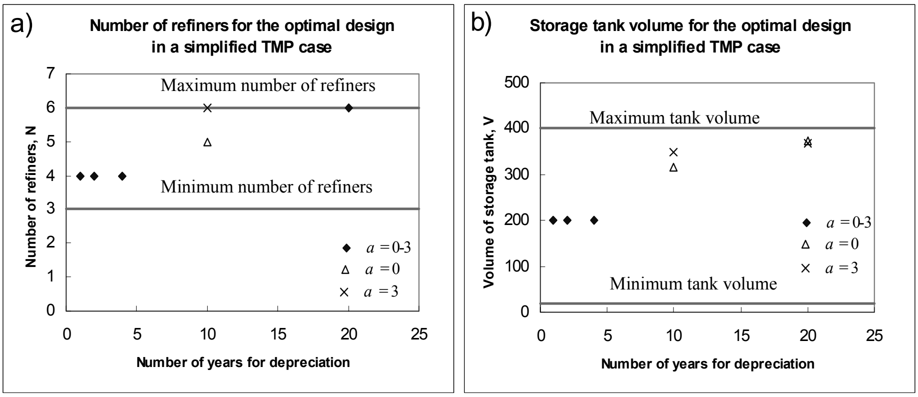


Figure 8. Risk premium weighting effect (a = 0 to 3) on the optimal design in the simplified TMP case with different number of years for depreciation: (a) number of refiners and (b) storage tank volume.

Design with the *worst case scenario analysis* (Suh and Lee 2001). The best robust solution was chosen amongst the design alternatives represented with Pareto optimalities, Figure 9. The discrete cost function $C = f(V_{\mathrm{tank}})$ was modelled to a continuous one and the Pareto curve was established for the decision-making procedure. Thus the best robust solution was found nearest to the ideal point.

In Figure 9 point E stands for the stochastic model solution, and point W stands for the worst case analysis solution. $\overline{C}^{S}$ and C_w^{R} are the expected cost of the stochastic model solution and the worst case cost of the worst case analysis solution, respectively. X axis describes how far the solution is from the ideal solution of the stochastic model (X=0) and Y axis describes how far the solution is from the worst case (Y=0). The ideal point stands for the reference point for decision-making, the optimum with the conflicting objectives (robustness and optimal stochastic model solution) is found as the nearest point to origin.

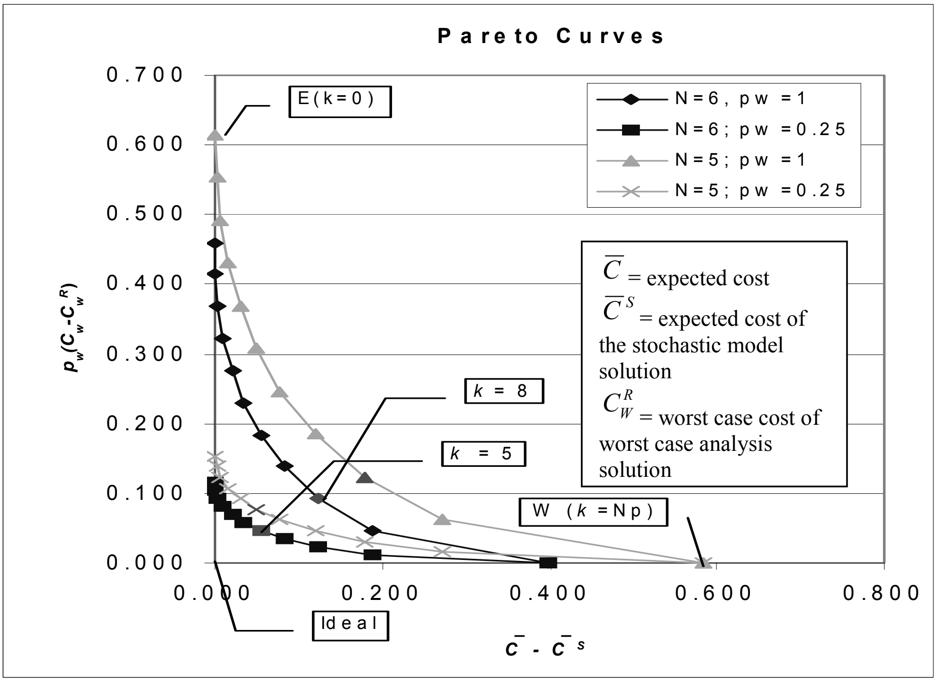


Figure 9. Robust optimization of the simplified TMP case with four different demand scenarios of the paper machine. The best robust solutions based on the worst case analyses are found with N = 6 and with the indices k = 5 and k = 8 for the different scaling factors (probability of the worst case scenario) $p_w = 0.25$ or $p_w = 1$ (no scaling), respectively.

Comparison of the design principles. The results of the risk premium study were compared to the robust solution of optimal design of the TMP plant in Table 6.

For the TMP design case, the stochastic model gives $N = 5$ refiners for the optimal design. Both the risk premium study and the robust optimization study prefer $N = 6$ refiners in decision-making. The optimum storage tank volume is 350 units, while the stochastic model suggests 9% smaller volume for the tank. Note that the design optimization with a stochastic model does not take into account any uncertainty in design, but only external factors (production demand).

Table 6. Design alternatives for the simplified TMP case with the 10 years of depreciation time for the capital costs. (a=risk premium weighting factor)

Design parameter	***Stochastic model***	***Risk premium***		***Robust optimization***		
		a = 3	*a* = 0	worst case		decision
Number of refiners, N_{Ref}	5	6	6	5	6	6
Volume of tank, V_{tank}	318	349	349	299	337	349
Costs (m = 10)	983	1104*	996	1214	1212	993

*The total costs in the risk premium study include the extra cost for the risk.

Conclusions. The TMP design alternatives are based on the overall feasibility region of all scenarios. However, if one of the scenarios strongly restricts the feasibility region and, in addition, is quite infrequent, the scenario can be omitted from the optimization. This might cause a situation where the TMP line is temporarily unable to produce pulp for the paper mill. The question then is, what will be the additional cost of such a scenario, and more generally, how the extra cost should be handled in design optimization. Although the TMP case dealing with uncertainty was carried out on a conceptual design level (the production capacity increase in the long time period was not included in the case calculations for instance) applying the risk premium and the new robust optimization approach (Suh and Lee 2001), the study reveals facts to be considered in real TMP plant design. To the authors' knowledge, a similar study has not been published earlier.

9.1.2 Measurement uncertainty

Paper VII presents how a scenario-based approach in simultaneous control and process design may give valuable new information on process characteristics under uncertainty. In the paper machine basis weight control study measurement uncertainty plays an important role. In the cascaded approach, consistency (that affects the basis weight together with filler and broke feed) is measured at an earlier process stage, at the paper machine headbox, whereas the current practice is to measure the basis weight at the end of the process. The possibility to react earlier based on the headbox consistency measurement gives potential to a more accurate basis weight control, but the applicability of this cascade control structure depends on the headbox consistency measurement accuracy, which is strongly hampered by the measurement noise. This approach is compared in different control alternatives (PI, MPC, Dahlins algorithm).

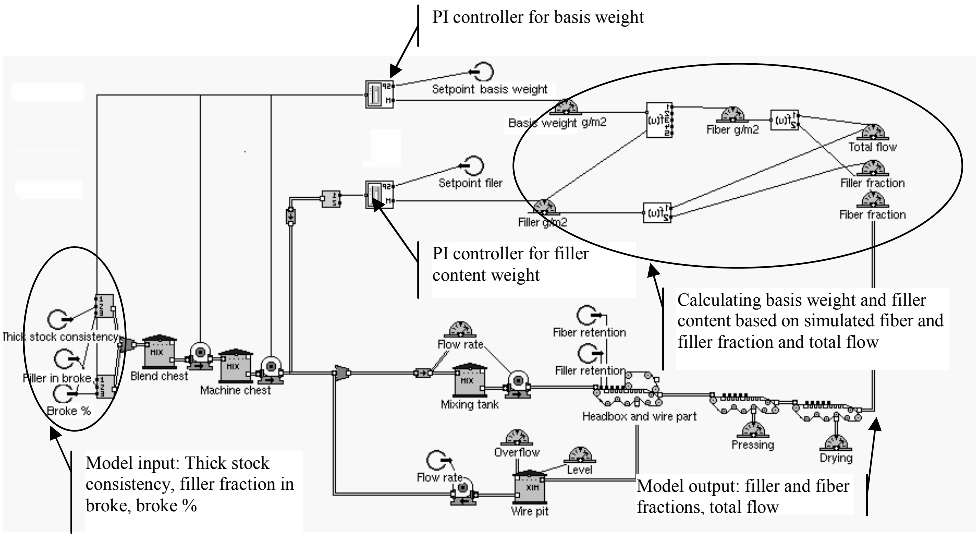


Figure 10. Simulation model with two PI controllers. The control loops are one for filler content and one for basis weight.

Case process. The papermaking process consists of mixing, dilution, and separation stages with rather little chemical action. In this analysis, the role of chemicals is neglected and the process is thus described as purely physical system. The subprocesses of the papermaking process are (see also Figure 10):

- Pulp preparation, mixing of water and fibers
- Dilution, web forming, and water removal
- Pressing and drying sections remove the remaining water

The essential measurements of the process are the fiber and filler consistencies before the wire section and in the wire pit as the well as basis weight and filler content of the ready-made paper. To actuate the process, there are two manipulated variables: a thick stock valve after the mixing chest determining the amount of undiluted main fiber flow to dilution point and a filler valve determining the fresh filler dosage at the dilution point.

Two *potential control structures* exist, direct control based on basis weight and filler content measurements after the drying section, or cascaded control where the inner loop regulates the consistency before the wire section and the outer loop gives set points to consistency measurements based on basis weight and filler content measurements after the drying section. Cascaded control is hampered by the high uncertainty in the measurement, and different noise levels (sensor accuracy) are included in the study.

Scenarios. To take into account external factors, scenarios concerning the external future environment of the system need to be specified. The disturbance scenarios are strongly specific to the paper grade and machine. First it was checked whether all the disturbances considered; the retention chemical change, grade changes, broke percentage and broke filler consistency, can be controlled by using at least some of the potential control solutions. It was also noticed that the optimal selection of the control structure depended on the frequency of different disturbances. The disturbances considered were all included in one scenario, see Table 7.

Table 7. Disturbance scenario

Time	*Disturbance*
150	Retention chemical change, retention increases 10% (now filler 55%, fiber 85%)
500	Grade change (new setpoints basis weight 50 g/m^2, filler 2 g/m^2), retentions change (now filler 60% fiber 93%)
1000	Grade change (new setpoints basis weight 45 g/m^2, filler 2.5 g/m^2), retentions change (filler 55% fiber 88%)
1500	Broke filler consistency starts to increase, thick stock consistency drops to 0.017%
2000	Broke % increases to 45, broke filler consistency reaches level 0.0014 and stays there.
2500	End of scenario

Several objective functions were calculated; the ratio of off-specification and in-specification production was minimized (index 1), the profit defined as a value of production minus cost due to off-specification production was maximized (index 2), costs due to off-specification production, process equipment and instrumentation (index 3) as well capital costs due to wire pit construction were considered (index 4). However, index 3 was dominated so strongly by capital costs that it was omitted. In index 4a only controller and instrumentation costs are taken into account, in index 4b the chest alternatives and their costs also are included.

An optimization problem includes controller selection and tuning as well as blend and machine chest sizing. The other process variables are assumed to have constant cost and performance values. Utility costs are assumed to be constant in all scenarios and process designs.

Conclusions. Results (Figure 4 in Paper VII) show that the cascade controller becomes optimal when the uncertainty σ in consistency measurement is below roughly 0.00007, which is to be compared with the average measured value of 0.002. The cascade controller becomes optimal roughly at the same value of standard deviation regardless of which performance index is employed. The results depend on capital costs, the price of the end product, the cost of off-specification production, and scenarios.

It is obvious that if the consistency measurement uncertainty can be reduced under 0.00007, a considerable economic gain can be achieved, since all economic indicators improve. Taking into account the high added-value per time in papermaking, high development costs of such a sensor would be justified.

9.2 Stochastic simulation approach

Paper VIII presents a stochastic simulation approach to handle uncertainty in control design caused by paper machine breaks and run lengths. Stochastic (Monte Carlo) simulation is a well known approach, in which all the probabilistic data is described as cumulative probabilities, and then a random number generator is used to draw samples from these probability distributions. This approach randomly generates values for uncertain variables over and over to simulate a model. The results can be expressed as a frequency distribution (Rose 1976).

Stochastic simulation has been widely applied in process engineering, for instance in determining process performance, when operating conditions and equipment reliability are varied (Gaddy and Culberson 1973). Lately dynamic stochastic simulation has also been applied to heat exchanger design. The approach represented the real operation conditions better than the original calculation within the bounds of the assumptions made, and gave a more reliable basis for decisions (Knetsch and Hauptmanns 2005).

In papermaking predicting the exact occurrence and duration of a single break is impossible or extremely difficult. However, nowadays data from the process is collected and stored automatically to history databases. This readily available data can be used for defining probability distributions for run and break lengths.

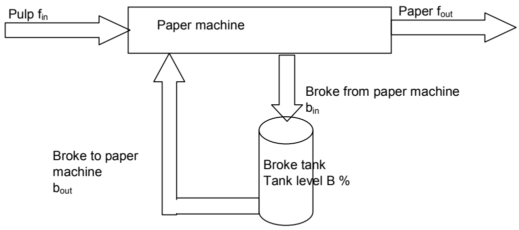


Figure 11. Simplified paper machine broke system

As paper machine speeds increase and printing technologies develop a uniform paper quality has become more and more important. Therefore, stochastic disturbances, caused by broke tank inflow to the paper machine wet end, affecting the paper quality need to be carefully minimized. Because the occurrence of a single break is impossible to predict, statistical analysis is useful when comparing the process behaviour in different control schemes. Controlling this stochastic disturbance optimally requires process knowledge and a careful tuning and selection of a controller. So far the broke tank level control problem has been widely studied, but to the authors' knowledge stochastic simulators have not been utilized in selecting the optimal controller tuning, only for defining the hard constraints for the broke tank outflow maximum value and maximum change (Ogawa 2004). In Paper VIII a new application, where the stochastic features are included in the simulator when tuning the applied non-linear P controller, is presented.

9.2.1 Uncertainty in paper machine run time and break distributions

In papermaking controlling the broke tank level has strong effect on wet end stability. The broke tank level is usually controlled manually or by a single PI controller and the stochastic nature of the inflow disturbances are not taken into account. In this averaging level control problem, fluctuations in the outflow need to be minimized while keeping the tank level within acceptable limits. In the study presented in Paper VIII, non-linear P controller performance and its tuning are studied with a stochastic simulator and compared to real mill data.

Defining the stochastic features. The data for the background study for the example application (Figure 11) was collected from a mill for a period of one year with the sampling rate of once a minute. Different distributions were considered. In the literature, exponential distributions were fitted for run time and break length distributions with varying success (Ogawa et al. 2004, Khanbaghi et al. 1997). Based on our current data, Weibull distribution fits for run time distribution surprisingly well. The χ^2 tests, see Table 1 in Paper VIII, show that different grades could be described using only a few different parameter sets in the Weibull distribution. The grades used in our example are defined with Weibull parameters

Grade A: η =1, σ = 180
Grade B: η = 0.6, σ = 120

With both grades the average run time is 3 hours and the parameters for log-normal break length distribution are μ = 2.35 and σ = 0.35. These parameters give an average break length of 10 minutes, which is realistic when shut-downs or the like are excluded from the mill data.

Cost factors. The task of a broke tank is to prevent stochastic changes in feed flow from disturbing the process conditions in the paper machine wet end. Therefore, following the broke tank level set point is not alone a useful criterion in the broke tank level control, but also the outflow from the broke tank should change as smoothly as possible not to create extra fluctuations. On the other hand, the tank should be run rather empty during normal operation to avoid overflows, when breaks occur. Therefore, penalties for running the tank empty or overflow are also needed.

The stochastic properties, for example standard deviation, can be used in describing the smoothness. For instance, when the production plan has been defined, the stochastic simulator can be run for a thousand times and the standard deviation of the tank outflow and level can be calculated at each time point or for each simulation.

Non-linear P controller (NLP). The simulator uses a nonlinear P controller where the controller gain depends on the operating point. The flow out from the broke tank is calculated as:

$$b_{out} = \left(b_{out}^{(\min)} + \frac{B - B^{(\min)}}{B^{(\max)} - B^{(\min)}} \left(b_{out}^{(\max)} - b_{out}^{(\min)} \right) \right) \frac{f_{in}}{100} \tag{7}$$

where $b_{out}^{(\max)}$ $\in [11\ 30]$% of total fibers
$b_{out}^{(\min)}$ $\in [1\ 10]$% of total fibers
$B_{out}^{(\min)}$ = 20% tank level
$B_{out}^{(\max)}$ = 80% tank level
B = broke tank level, %
b_{out} = flow out from the broke tank (t/h)

Because the actual tank level has minor importance as long as no overflows occur, it is obvious that bigger control actions can be allowed near the upper and lower limits. The minimum and maximum values of $B_{out}^{(\min)}$ and $B_{out}^{(\max)}$ were defined a priori based on general process knowledge.

Tuning the NLP controller with a stochastic simulator. To tune the control parameters $b_{out}^{(\min)}$ and $b_{out}^{(\max)}$, the stochastic simulator is run 10,000 times with all allowed parameter combinations. A simulation time horizon was chosen to 1,000 minutes for convenience. Since the initial tank level has a strong effect on the probability of overflow, simulations with two different initial tank levels (20% and 80%) were calculated. The variation in the broke feed is minimized while keeping the joint probability of running empty or full under 1% (i.e. 100 times of 10,000). In Figure 4 in Paper VIII, the effect of control parameters on the probability of running the broke tank empty or full from initial tank levels 20% and 80% are demonstrated together with a broke feed deviation. The optimum is found for grade A with $b_{out}^{(\min)}$ = 7% and $b_{out}^{(\max)}$ =18% while for grade B with $b_{out}^{(\min)}$ = 7% and $b_{out}^{(\max)}$ =26% . This result is natural since grade B, having a lower shape factor, is more unstable in the beginning of a run. To overcome this, a higher $b_{out}^{(\max)}$ is needed to decrease the tank overflowing probability.

Results and comparison with mill data. To compare the simulations with real mill data, the simulator was run with a real break signal and two sets of control parameters:

- the optimum $[b_{out}^{(\min)}, b_{out}^{(\max)}, B_{out}^{(\min)}, B_{out}^{(\max)}] = [7\ 18\ 20\ 80]$
- alternative control strategy $[b_{out}^{(\min)}, b_{out}^{(\max)}, B_{out}^{(\min)}, B_{out}^{(\max)}] = [5\ 10\ 10\ 90]$

The break signal, simulated and real tank level, and flow from the broke tank are presented in Figure 12 and Figure 13. As can be seen in Figure 13, the NLP control result is much smoother, and smaller disturbances to the downstream process and paper machine feed are caused than with the current practice. Also, an alternative control strategy that produces even smoother broke feed is presented in Figure 13, but a simulation reveals that the probability of tank overflow is 3% for grade A and 10% for grade B, when the initial tank volume is 50%.

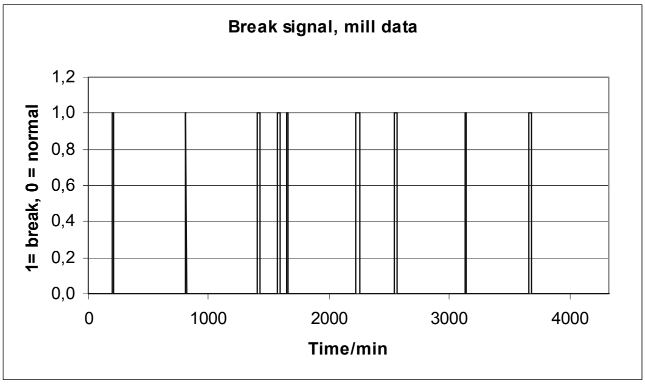
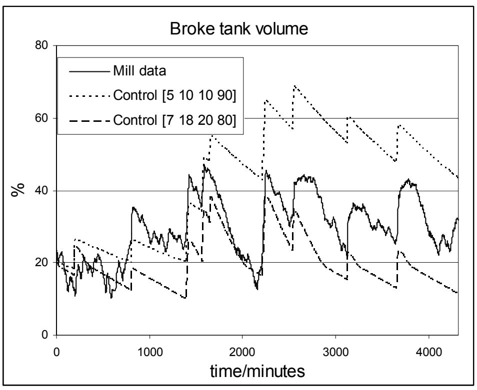


Figure 12. Real break data used for comparisons



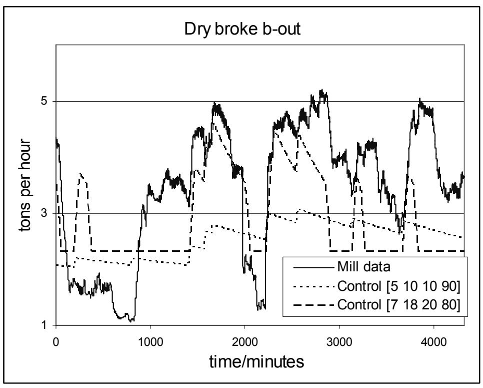


Figure 13. Broke tank volume and broke flow to paper machine, simulated and mill data

Conclusions. In Paper VIII stochastic distributions were fitted for break and run lengths and utilized for tuning optimally a non-linear P controller for broke tank level. By using confidence interval tests, it was found that grade dependency should not be neglected.

This approach made it possible to simulate realistic stochastic features of the process in a reasonable time. The controller tuning is selected based on the downstream process requirements, and compared with the mill data. The NLP control provided a smoother control than the current situation. The presented approach provides a starting point for more rigorous control studies.

10 Conclusions

The challenge in design is to create a process or equipment for future needs. The changing world and competition bring about challenges, such as a shorter project time, the utilization of earlier experience, a need for creative design and organizational learning as well as robust design under uncertainties. The thesis presents new methods to answer the challenges. Case-based reasoning (CBR) provides a method for fast process and equipment design by utilizing earlier knowledge systematically. The main benefit of CBR applications is that readily available knowledge can also be utilized systematically in large and complex problems like the separation process synthesis and design. In this way the time-consuming screening stage in a design project can be sped up for instance in separation process synthesis. The system learns by updating the information in the database. In fact, the system can function as an institutional memory and facilitate organizational learning in the company such as process equipment supplier. Therefore, the use of CBR enhances a systematic documentation practice and the reuse of experience. The continuous organizational learning process can be facilitated by the inclusion of design quality factors as parameters in cases. Creativity can be implemented by CBR searches by using analogies as presented.

The thesis presents a new approach to separation process selection and sequencing for both azeotropic and non-azeotropic distillations and other separation methods (Papers I to IV). The method is based on three main steps by CBR:

1) Selection of single separations (distillation-based and other separations)
2) Separation sequencing by using search criteria
3) Search for combined separation operation.

Equipment design can be enhanced by using information from earlier designs (as presented in Paper V). Especially suppliers who design the equipment partly based on experimental data may benefit from CBR systems since the system forms a design database that allows a systematic reuse of earlier designs and provides feedback from the success of the designs. The new method presented allows more realistic design, since the allowable alternatives of equipment parts are included in the reasoning.

However drawbacks in the CBR approach to process design exist. The needed case database needs to be extensive enough to provide the knowledge needed for the design tasks at hand. In case of difficult creativity requiring design task, different kind of searches can be made in database to support innovative design thinking. The interaction with the user is challenging; on one hand the system can be used for learning, but on the other hand the CBR approach is an expert tool, which requires expertise from the user in making useful queries. Also the system maintenance needs careful consideration. It has to be decided which cases are outdated, how their maturity changes are handled and how different case types can be added to the database.

A further challenge in design is how to create robust and flexible design capable of operating in changing situations. Three new applications are presented. For design under uncertainty, an application utilizes scenarios, risk premium and robust optimization approaches is presented with the uncertainty in the product demand of a thermo-mechanical pulp plant (Paper VI). Scenario-based simultaneous process and control design application is presented (Paper VII) with the uncertainty related to paper machine headbox consistency control measurement. Stochastic simulation has been applied to paper machine broke tank level control, where the uncertainty is due to paper machine breaks (Paper VIII). Studying systematically the effect of uncertainty in a future operating environment on process design may prevent unprofitable investments. The systematic studies, at their best, give also an idea how economic gain can be achieved. For instance, based on the measurement uncertainty study, it is obvious that an investment to a more accurate headbox consistency measurement would be highly profitable. The approaches also give means to weigh the risk and possible reward. For instance in the broke tank level control application, running the process smoothly increases risk of broke tank overflow, but also minimizes the process fluctuations and thus improves the product quality.

The presented approaches are complementary. CBR is very applicable at the early stages of the design process when data needed for modeling is not available and process alternatives need to be quickly screened to find the feasible ones for further studies. At later design stages the uncertainties can be taken into account by means of scenario or stochastic models to find optimal or near to optimal design. At this stage parameters needed for modeling are already fixed and the number of process alternatives limited. CBR is also applicable in detailed equipment design, where rigorous adaptation routines can be run automatically. The presented approaches complete each other; CBR is beneficial when the uncertainty is due to technical difficulties in defining process parameters or modeling the essential phenomena, whereas scenario based approaches are applicable when predictions about future events need to be included. When the uncertainties can be described by means of pre-defined distributions, the stochastic simulation may give the best results. These methods could even be combined to describe the effect of uncertainty or variation in CBR retrieval parameters on the CBR design results. This is however beyond the scope of this thesis and remains to be studied in the future.

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