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STUDIES ON COMPUTER-AIDED CONCEPTUAL PROCESS DESIGN

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ABSTRACT

Conceptual process design phase is of prime importance to the performance and the profitability of a new or retrofit process. It is also a highly complex task with a large number of process alternatives, a large variety of requirement specifications and large differences in temporal and spatial scales. Therefore, it is essential to continuously improve design methods. The research should not only be focused on modelling unit operations or processes but also to develop a framework to support design tasks during the lifecycle of the chemical process.

Main target of this thesis is to study and present methods how to intensify the conceptual process design phase. The newly developed methods and tools are applied to process equipment selection and pre-design, separation process synthesis and process design support.

First, the theory of case-based reasoning (CBR) was studied with focus in applicability in process engineering. CBR was utilised for general separation process synthesis. The main phases of general CBR-based separation process synthesis algorithm consist of selection of the methods of single separations, selection of separation sequences and selection of combined (hybrid) separations. Selection of single separation also includes selection of azeotropic separations. The applicability of CBR in separation process selection and design was studied by building few prototype CBR systems.

The possibilities of CBR and object database techniques in chemical process engineering field have been illustrated by building applications for an inherently safer process design and for a heat exchanger selection.

A web-service based approach in conceptual process design, parameterised constructors, which are able to construct process and initial data for control system configuration is also introduced in the thesis. The preliminary process design task can be first defined in a more general level and as the design process proceeds; more accurate models (e.g. PI and control system diagrams, simulation models) are composed and used.

TIIVISTELMÄ

Käsitteellisen prosessisuunnittelun vaihe on erittäin tärkeä uuden tai uudistettavan prosessin suorituskyvyn ja tuottavuuden kannalta. Se on myös erittäin monimutkainen tehtävä johtuen lukuisista prosessivaihtoehtoista, vaatimusmäärittelyiden monimuotoisuudesta sekä tila- ja aikaskaalojen eroavuuksista. Tämän vuoksi on välttämätöntä, että prosessisuunnittelumenetelmiä jatkuvasti kehitetään paremmiksi. Tutkimusta pitäisi kohdentaa yksikköoperaatioiden ja –prosessien mallituksen lisäksi myös kemiallisen prosessin koko elinkaaren aikaisia suunnittelutehtäviä tukevan palvelukehyksen kehittämiseen.

Väitöskirjassa tutkittiin ja esitettiin menetelmiä, joiden avulla käsitteellistä prosessisuunnittelua voidaan tehostaa. Kehitettyjä menetelmiä ja työkaluja on sovellettu prosessilaitteen valintaan ja esisuunnitteluun, erotusprosessisynteesiin ja prosessisuunnittelun tukemiseen.

Työssä tutkittiin tapauspäättelyn teoriaa keskittyen sen soveltuvuuteen prosessisuunnittelussa. Tapauspäättelyä sovellettiin erityisesti erotusprosessien synteesimenetelmän kehittämiseen. Tapauspäättelypohjaisen erotusprosessisynteesialgoritmin päävaiheet koostuvat yksittäisen erotuksen valintamenetelmistä, erotusjärjestyksen valinnasta ja yhdistettyjen (hybridi) erotusten valinnasta. Yksittäisen erotuksen valintamenetelmä sisältää myös atseotrooppiset erotukset. Tapauspäättelyn soveltuvuutta erotusprosessin valintaan tutkittiin rakentamalla muutamia prototyyppisovelluksia.

Oliokantatekniikan ja tapauspäättelyn etuja demonstroitiin rakentamalla luontaisesti turvallisemman prosessin valintajärjestelmä sekä lämmönsiirtimen esisuunnittelusovellus. Olemassa olevia esimerkkitapauksia voi käyttää hyväksi uusien samankaltaisten ongelmien ratkaisuissa.

Väitöskirjassa käsitellään myös prosessisuunnittelun lisäarvopalveluita, parametrisoituja muodostimia**,** jotka pystyvät eri tilanteissa muodostamaan prosessi- ja automaatiokonfiguraatio lähtien suunnittelijan antamista korkeamman tason vaatimuksista. Suunnittelutehtävä määritellään ensin yleisemmällä tasolla. Suunnitteluprosessin edetessä prosessisuunnittelun lisäarvopalveluiden avulla muodostetaan ja käytetään tarkempia malleja (esim. PI- ja säätökaavioita, simulointimalleja). Päätarkoituksena on rutiinisuunnittelun tehostaminen, automaatiotoimintojen (tyyppipiirikuvauksien), ajotapadokumenttien sekä automaatiosuunnittelun lähtötietojen generointi. Tavoitteena on suunnittelukulttuurin muutos ja osoittaa, miten uutta suunnittelukulttuuria voidaan toteuttaa prosessi- ja automaatiosuunnittelun kannalta.

PREFACE

The research described in this thesis was done in the Laboratory of Chemical Engineering and Plant Design in Helsinki University of Technology during 1999-2005.

I am very grateful to my supervisor Prof. Markku Hurme for his guidance and support in this work and for his help in preparing the final thesis. I also thank my co-authors for co-operation and advices.

Espoo, July 2006

Timo Seuranen

LIST OF PUBLICATIONS

This thesis is based on the following publications (Appendices I-VII), which are referred to in the text by their roman numerals:

I. Pajula, E., Koiranen, T., Seuranen, T., Hurme, M., Computer aided process equipment design from equipment parts, *Comput. Chem. Eng.* **23** (1999), Suppl. S683-S686.

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

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

IV. Seuranen, T., Pajula, E., Hurme, M., Applying CBR and object database techniques in chemical process design, *Lecture Notes in Artificial Intelligence*, Vol 2080, 731-743, 2001.

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

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

VII. Seuranen T., Karhela T., Hurme M., Automated process design using web-service based parameterised constructors, *Computer-Aided Chemical Engineering*, Vol 20, 1639-1645, 2005.

Timo Seuranen’s contribution to the appended publications

I. The author participated in the definition of research plan and writing of the manuscript together with the co-authors.

II. The author participated in the methodology development and writing of the paper together with the co-authors.

III. The author participated in the CBR application development, the definition of research plan and wrote the manuscript together with the co-authors.

IV. The author has full responsibility in writing the manuscript and publication. The author has programmed both applications presented in the paper. Elina Pajula and Prof. Markku Hurme have commented on the paper.

V. The author was responsible for definition of the research plan, wrote the manuscript together with the co-authors, and prepared the final paper.

VI. The author participated in the definition of research plan and wrote the manuscript together with the co-authors.

VII. The author has full responsibility in writing the manuscript and publication. Dr. Tommi Karhela and Prof. Markku Hurme have commented on the paper.

STUDIES ON COMPUTER-AIDED CONCEPTUAL PROCESS DESIGN

NOTATION

Symbols

D	distillate flow rate
F	feed flow rate
f	percentage concentrations of the component pair
L	reflux rate
N_{real}	number of real stages
N	the number of components in the separation problem
R	reflux ratio
R_{min}	minimum reflux ratio
S	separation factor
V	vapour flow
x	bottom product
y	distillate
z	feed composition of components lighter than the heavy key

Greek letters

a	relative volatility
$\bar{a}$	mean relative volatility
h	tray efficiency

Subscripts

H	heavy key
L	light key

Abbreviations

CES	Coefficients of ease of separation
CBR	Case-based reasoning
DMF	Dimethylformamide
HK	Heavy key
LK	Light key
MINLP	Mixed integer non-linear programming
MSA	Mass separation agent
PID	Piping and instrumentation diagram
THF	Tetrahydrofuran
XML	Extended mark-up language

1. INTRODUCTION

The products of the chemical industry can be found everywhere in our modern society. Besides typical products like petrochemicals, industrial gases, plastics and solvents, the chemical industry also produces a large variety of products: pharmaceuticals, food additives, paint and detergents, many other chemical and biochemical products, etc. The basic function of chemical processes is that feedstock is converted into products that satisfy certain societal needs (Seider et al. 1999). Conversion can be the seemingly simple process or it can also be a highly complex process containing multiple chemical reactions, recycles and separation stages. During the last decades, chemical processes have become increasingly complex. Following three reasons have led to this increasing complexity (Ogunnaike 1996): 1) the continuous drive for more consistent attainment of high product quality, 2) more efficient use of energy and 3) tighter safety and environmental regulations.

The preliminary process design has very crucial importance for the performance and the profitability of a new or retrofit process. Therefore, it is essential to continuously improve design methods and access the resulting economical and environmental opportunities. The ongoing research should not only be addressed a particular unit operation or an integrated process but also aims at developing new methods and tools and even a whole process design framework to support design tasks during the lifecycle of chemical process.

Conceptual process design is a highly complex task. Therefore, systematic methods for conceptual process design are required. The following characteristics of conceptual design contribute to this complexity (Meeuse 2002):

- A large number of process alternatives are possible.
- A large variety of requirement specifications should be satisfied.
- Large differences in temporal and spatial scales are involved.

The main target of this thesis is to study and present methods for intensifying the preliminary process design phase. The newly developed methods and tools are applied to process equipment selection and pre-design, separation process synthesis and process design support systems.

2. CONCEPTUAL PROCESS DESIGN

2.1 Introduction

Conceptual design is the entire process of investigation of the problem including the discovery of possible barriers to the required task, systematic generation of feasible process alternatives and analysis of the process alternatives so that the best one is chosen based on the available information. Douglas (1988) has given a definition for conceptual design: *to find the best process flowsheet (i.e., to select the process units and the interconnections among these units) and estimate the optimum design conditions.* Biegler et al. (1997) and Seider et al. (1999) have given similar definitions.

Conceptual design operates on very limited information that is available in the early stages of a project, has to happen quickly, often has to be done pre-award and thus cannot cost too much. Ideal conceptual design provides, in the allotted time, a final design of the project result to sufficient detail for accurate and concurrent time and cost estimates. If compared to detailed design, only a limited number of people are available for conceptual design phase. Conceptual design also requires personnel with the highest level of expertise.

The importance of conceptual process design becomes clear when one realizes that, although a relatively small fraction of the total budget is spent during the conceptual design, the majority of investment costs are assigned in this phase. In fact, the conceptual design stage for a new commercial process costs usually 10-20 % of the total development cost, but these decisions fix 80 % of the total project costs (Douglas 1988). Another problem is that less than 1 % of ideas for new process designs become commercialised. Therefore, a large number of concepts need to be evaluated rapidly, cheaply and with sufficient fidelity. Douglas (1988) has estimated that for a typical design the number of alternatives that might accomplish the same goal can be over 1 billion. Out of these alternatives one aims to select the best ones, which meet the objectives, e.g. the design with the lowest financial costs that satisfies all other constraints. The main difficulty with this large number of alternatives is that the path from design decisions to the demands to be satisfied is complex and non-linear. This requires systematic methods to reduce the number of alternatives early in the design process.

2.2 Stages of conceptual process design

Figure 2.1 divides the process synthesis step into several subtasks. After problem specification in *concept generation* step different process concepts on which to base the design will be identified. Next in *generation of alternatives* step any available information will be inspected thoroughly to find existing processes or to develop new ones. In *analysis* step each process alternatives will be analysed by calculating e.g. mass and energy balances to find out different flows, temperatures, pressures, etc. In the next step, process‘s performance will be *evaluated*. In *optimization* step, the design will be improved by adjusting and refining the decisions made in previous steps. (Biegler et al. 1997)

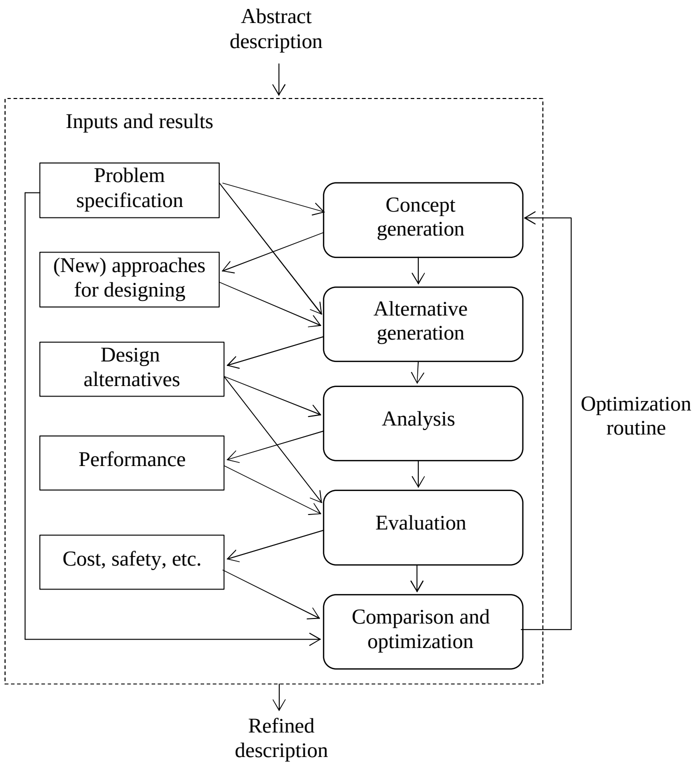

Figure 2.1 The steps of process synthesis (modified from Biegler et al. 1997)

2.3 Criteria for process design

In process design, the designer has to cope with a large variety of requirements. Some of these are explicitly state in the Basis of Design, others not. Herder and Weijnen (1998) have defined quality criteria for process design based on industrial case studies and expert panel meetings. These criteria were seen as the most important quality criteria in industrial practice. Figure 2.2 shows structured summary of criteria divided into design quality criteria and design process quality criteria. The safety, operability and environmental performance were very important criteria for most participants.

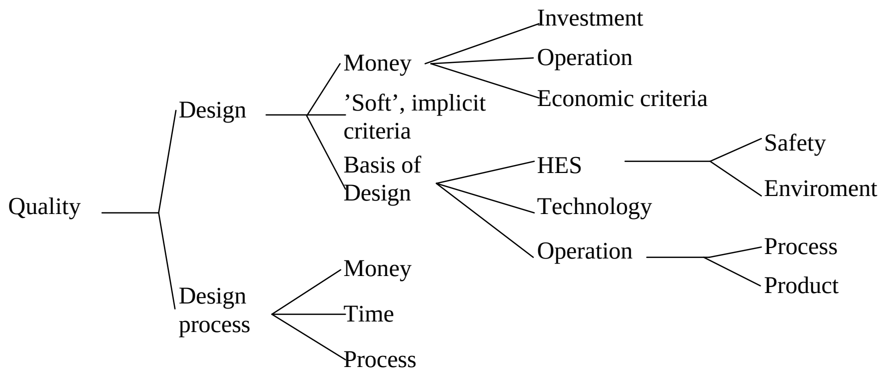

Figure 2.2 Classification of quality criteria (Herder and Weijnen 1998)

All those criteria mentioned above are regarded nowadays as relevant, but it is very hard to consider all of them during the decision-making in the conceptual design phase, especially since the different criteria play a role at different phases in the design. The problem is that the route from a design decision to the quality factor is quite complex, comprising many causal steps and having non-linearity behaviour. Therefore, a challenge for conceptual process design is to know when which quality factors should be considered and how the design decisions made have an influence on these quality factors. (Meeuse 2002)

2.4 Project/engineering steps

Conceptual design is a part of the overall chemical innovation process, which leads from the problem identification to the construction and operation, i.e. the sequence is identification, chemistry development, process design, plant design, detailed engineering, equipment fabrication, plant construction, commissioning and operation. Similarly, the process design activity within the innovation process includes the sequence of goal and objective formulation and then the synthesis, analysis, evaluation, and selection among process alternatives to achieve the goals. Optimal selection among alternatives depends in part on how each alternative might be implemented by all the stages yet to follow. Later steps are better defined but have a lesser impact on overall economics. Conversely, earlier steps are poorly defined but decisions made have a greater impact on overall process success. (Siirola 1996)

2.5 Process design methodologies

The current challenges to the chemical process industries include quicker development of new products and processes, finding new chemical routes to existing products and making existing processes more efficient. The challenges will not only require sustaining the existing approaches, but also will demand new approaches to process design and development. Nowadays, new process synthesis methods have to take into account a greater number of aspects, such as more effective representations of the underlying physical sciences and engineering art, new social concerns, new design strategies, and new computerized implementations. This will expand the role of the systematic generation process synthesis paradigm and increase the interdependency with process and operability and control expertise. (Barnicki and Siirola 2004)

The existing chemical process design approaches can be divided to: (Paper IV)

1. Heuristic and engineering experience based methods, which use often a hierarchical approach (Douglas 1988, Smith 1995).
2. Optimisation approaches using either mixed integer non-linear programming (MINLP) (Grossmann and Kravanja 1995), genetic algorithms (GA) (Khalil 2000), and simulated annealing (Faber et al. 2005).
3. CBR methods where existing design cases are reused and adapted to solve new design problems. This approach has been used to some extent to equipment design in chemical engineering but very little to process design.

The problem in heuristic approaches is that no computer-based systems are usually available to support them. Therefore, the approach relies totally on the designer. This is opposite to the optimization-based approach, which relies on computerized calculations. The main idea of it is to formulate a synthesis of a flowsheet in the form of an optimisation problem. It requires an explicit or implicit representation of a superstructure of process flowsheets, among which the optimal solution is selected. However many design criteria such as safety or operability are difficult or impossible to quantify explicitly. The use of optimisation requires that the alternatives have to be limited by the user. Therefore, the main differences of the approaches are related to the interaction with the user, requirement of superstructure and the possibility of combinatorial explosion. In

MINLP and GA, a superstructure is required for the optimisation algorithm. To our experience the differences of methods can be summarized as in Table 2.1.

Table 2.1 Comparison of chemical process design approaches (Paper IV).

	MINLP	GA	CBR
superstructure required	yes	yes	no
combinatorial explosion	yes	some	no/partial
non-interactive method	yes	yes	no

2.5.1 Knowledge-based methods

The knowledge-based methods include:

Case-based reasoning: CBR imitates human reasoning and tries to solve new problems by reusing solutions applied to past similar problems. This method is described in this thesis in more detail.

Rule-based systems: A rule-based expert system represents heuristic knowledge in the form of rules, such as IF–THEN. The rule can be used to perform operations on data to inference in order to reach appropriate conclusion (Liao 2005).

Mean-end analysis: The mean-ends analysis paradigm starts with an initial state and applies transformation operators to produce intermediate states with fewer differences until the goal state is reached. The mean-end analysis approach was used as an early systematic process synthesis method for overall process flowsheet synthesis (Siirola 1996).

Phenomena-driven design: The main idea is that: Process is control of physicochemical phenomena for a purpose. The methodology can be stated by 1) Can the phenomenon be controlled in certain boundary and 2) Can the phenomenon be controlled profitably and safely (Pohjola, 1997).

Phenomena based approach: The principle of the method is to identify and manipulate the process phenomena for novel process concept generation. The method is based on three-stage procedure: 1) process analysis, where all relevant phenomena and are identified, 2) development phase, where process phenomena are analysed and manipulated, and 3) generation of intensified process alternatives (Rong et al. 2004).

Conflict-based approach (CBA): The method is based on the TRIZ approach, which is a method for the identification of the system's conflicts and contradictions for the solution of inventive problems (Altshuller 1998). *CBA* decomposes a design problem into sub-problems. The method is used for modifying the solution space and screening alternatives at preliminary design stage (Li et al. 2002).

Driving force method: Process design should be optimised by the equal distribution of the driving forces throughout the process by assuming that the rates of entropy production are proportional to the square of the driving forces (Sauar et al. 1996).

Axiomatic design: The purpose is to define both a design methodology and a set of rational criteria for decision making (Suh 1990).

Evaluative approach: This method is based on combining best properties of existing process alternatives (Cziner et al. 2005).

2.6 Current trends in process design

There has been progress in the tools for conceptual process design in the past three decades. Conceptual design cannot only help the development of an economically desirable manufacturing process, but also can provide key competitive advantage e.g. faster time to market and new product formulation Pisano (1997). New developments are also expected in the process models for unit operations, prediction of property-structure-value relationships, phase behaviour, and systematic methods for simultaneous product and process design.

Product and process design

The increasing interest has risen for developing new design methodologies for chemical processes that are defined by their properties and performance. An approach based on Douglas's hierarchical procedure was published by Meeuse et al. (2000) for the conceptual design of processes for micro structured liquids. Dhingra and Malone (see Dhingra, 2001) used the attainable region theory to a laminar emulsion for determining feasible drop size distributions that are independent of the mixing equipment used. These provide targets for the mixing equipment configuration and help in generating system alternatives.

Phenomena based design

Process systems are beginning to construct at a more fundamental level by thinking processes as combinations of transport processes and phenomena. This approach will lead to designing not only the processes but also the unit operations themselves that should form the basis of these processes (Westerberg, 2004).

Design for controllability and operability

More complex systems can be mathematically modelled and solved with MINLP optimisation methods, e.g. with a sequential two-stage strategy for the stochastic synthesis of chemical processes in which flexibility and static operability are taken into account (Pintaric and Kravanja 2004). A simultaneous process and control design methodology is increasingly developed to advance towards the integration of process design, process control and process operability, e.g. approach based on novel mixed integer dynamic optimisation algorithms, high fidelity process dynamic models, conventional PI control schemes, explicit consideration of structural process and control design aspects, and explicit consideration of time-varying disturbances and time-invariant uncertainties (Sakizlis et al. 2004).

Concurrent design

Design processes in chemical engineering are also developed further, e.g. management system for dynamic and inter-organizational design processes (Heller et. al. 2004). Because design processes are highly creative, many design alternatives are explored, and both unexpected and planned feedback occurs frequently. Therefore, it is difficult to manage the workflows in design processes. One approach to manage design processes is the web-service framework, which supports the progress of a new kind of design culture (Kondelin et. al., 2004).

3. CASE-BASED REASONING

3.1 Introduction

Case-based reasoning (CBR) imitates the human thinking trying to solve new problems by using previously successful solutions to similar problems and adapting proven solutions to a current problem. The method uses systematically most similar existing problems and their solutions to create a solution to a current problem (Kolodner 1993). CBR does not require an explicit domain model. Implementation is reduced to identifying significant features that describe the case, an easier task than creating an explicit model. Furthermore, CBR systems can learn by acquiring new knowledge as cases (Watson and Marir 1994).

According to Aamodt and Plaza (1994) the central tasks that all case-based reasoning methods have to deal with are: identifying the current problem situation, finding a past case similar to the new one, using that case to suggest a solution to the current problem, evaluating the proposed solution and updating the system by learning from this experience. The processes involved in CBR can be represented by a schematic cycle (see Figure 3.1). CBR is typically described as a cyclical process comprising the four REs:

1. RETRIEVE the most similar case or cases.
2. REUSE the information and knowledge in that case to solve the problem.
3. REVISE the proposed solution.
4. RETAIN the parts of this experience likely to be useful for future problem solving.

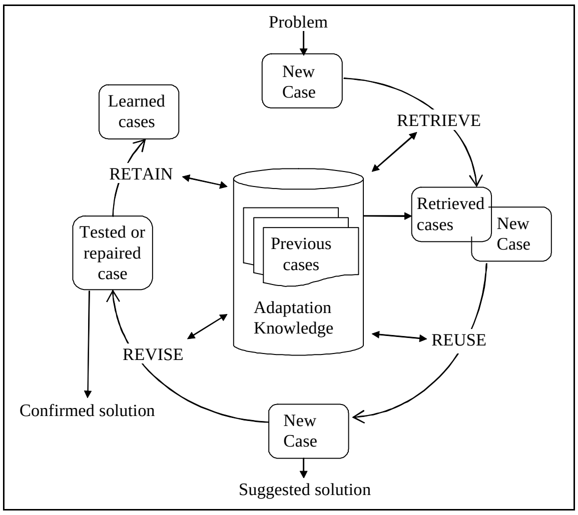

Figure 3.1 CBR cycle (Vong et. al 2002)

3.2 Properties of CBR models

Case-based reasoning methods have some characteristics that distinguish them from the other knowledge-based approaches. A typical case is usually assumed to have a certain degree of richness of information contained in it, and a certain complexity with respect to its internal organisation. Case-based methods are also able to modify, or adapt, a retrieved solution. Case-based methods utilise general background knowledge - although its richness, degree of explicit representation and role within the CBR processes varies. (Aamodt and Plaza 1994)

Rule-based systems have been the most commonly used approach to process synthesis. This kind of knowledge can also be included in a case-based reasoning system by defining “general cases” as presented in Paper III. For instance, if relative volatility is larger than 1.5 and the decomposition temperature is high for all components, the proposed separation method is distillation. The benefit of the general cases is that it gives always suggestion even if the specific application area is not well known beforehand or no near cases have been stored in the case base (see Figure 3.2).

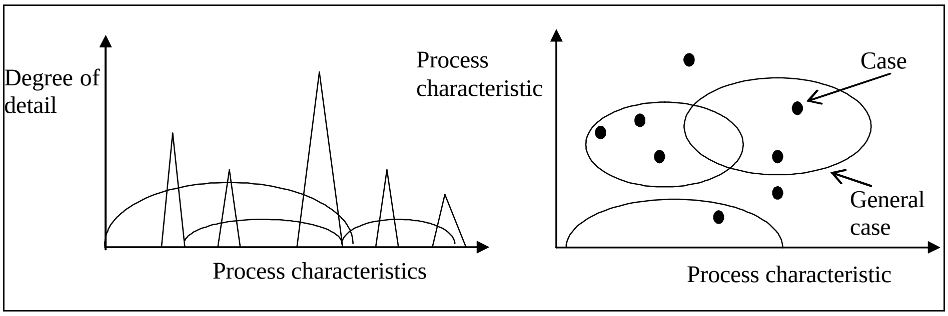

Figure 3.2 Structure of the case base with detailed and general cases (Paper III)

3.3 Case representation

Case-based reasoning is heavily dependent on the structure and content of its collection of cases. The case representation problem in CBR is primarily: deciding what to store in a case, finding an appropriate structure for describing case contents and deciding, how the case memory should be organised and indexed for effective retrieval and reuse. An additional problem is how to integrate the case memory structure into a model of general domain knowledge, to the extent that such knowledge is incorporated. (Aamodt and Plaza 1994)

Representation of cases must also support a full range of data types and should be able to structure cases in ways relevant to the application domain, i.e. ordered symbol hierarchies, relationships between features and object-oriented inheritance (Watson and Marir 1995). Most of the CBR systems have applied object-oriented techniques for representing cases as done in Paper IV. Such representation technique is particularly suitable for domains in which cases with different data structures occur.

3.4 Case retrieval

A retrieval algorithm using the indices in the case-memory should retrieve the most similar cases to the current problem or situation. The retrieval algorithm relies on the indices and the organisation of the memory to direct the search to potentially useful cases. Several algorithms have been implemented to retrieve appropriate cases, for example: serial search, hierarchical search and simulated parallel search (Watson and Marir 1994). Methods for case retrieval are nearest neighbour (used in Paper I-V), induction (used also in Paper II, III, V), and knowledge-guided induction and template retrieval. These methods can be used alone or combined into hybrid retrieval strategies.

3.5 Case reuse

The reuse of the retrieved case solution in the context of the new case focuses on two aspects:

a) The differences between the past and the current case.
b) What part of a retrieved case can be transferred to the new case.

In simple classification tasks the differences are considered non-relevant while similarities are relevant. The solution class of the retrieved case is transferred to the new case as its solution class. Other systems have to take into account differences in aspect a) and thus the reused part aspect b) cannot be directly transferred to the new case. It requires an adaptation process that takes into account those differences. Existing cases can be reused by using past case solution or using the past method that constructed the solution. (Aamodt and Plaza 1994)

3.5.1 Adaptation models

Lot of research interests has been focus on adaptation and several adaptation techniques have been developed: Abstraction and respecialisation (a general structural adaptation technique) that can be used in simple adaptations and in a complex way to generate novel, creative solutions. Critic-based adaptation focus a critic looks for combinations of features that can cause a problem in a solution. Reinstantiation is used to instantiate features of an old solution with new features. Model-guided repair uses a causal model to guide adaptation (Watson and Marir 1994). The complexity of adaptation method increases from null adaptation over transformational approaches to generative approaches. Further using multiple similar cases for adaptation is called compositional adaptation (Wilke and Bergmann 1998).

The adaptation method can be based on fuzzy logic. The quality of adaptation depends on the correlation between the selected input and parameters to be adapted (Virkki-Hatakka et. al 1997). Kraslawski et al. (1999) have used adaptation method, which is based on rough sets. Model based adaptation methods have been used as described in Paper I and III. The adaptation in Paper I is made using process design equations, where problem and design data is used as inputs of design equations. Maher and de Silva Garza (1996) have used genetic algorithms as adaptation methods.

3.6 Case revision

The adapted solution can still be incomplete, because it is adapted according to the requirement of the new case and this solution may have inconsistency among its solution parts. The adapted solution can be further adapted based on the user feedback and additional meta-adaptation knowledge (Vong et. al 2002). The evaluation task is usually done outside the CBR system, since it involves the application of a suggested solution to the real problem. The adapted solution may be applied to a simulation program that is able to generate a correct solution (Aamodt and Plaza 1994).

3.7 Case retainment – learning

The confirmed solution is stored to the case base. Only solutions, which have contribution to the future reasoning of solutions i.e. which cannot be done by only the current cases in the case base, should be stored. If the cases in the case base are capable enough to cover the newly adapted solution, this new solution should not be stored in order to avoid inconsistency and redundancy. The CBR system learns by updating the information in the case base. Properties, which are important, are weighted and non-relevant properties are weakened. (Vong et. al 2002, Aamodt and Plaza 1994)

4. CASE-BASED REASONING IN DESIGN

Over 50 % the work done by the designers on a day-to-day basis is routine design that consists of reusing past design solutions (Moore, 1993). Therefore, CBR is effective and useful in problem domains where similar problems take place frequently. CBR is well suited for weak-theory domains where full mechanistic models are not available and which include experience-based knowledge. It is a suitable technique for searching in partially structured databases with information about different technical solutions applied in a company earlier. Since CBR is a methodology, which can be used in all types of design, there are many applications, for example in civil engineering, architectural, mechanistical design, and building.

CBR has a diversity of applications in various design problems: in manufacturing process design (Takahashi et al. 1995), in building and mechanical design (Rivard and Fenves 2000; Mileman et al. 2002), in material science (Amen and Vomacka, 2001; Mejasson et al. 2001), in fault diagnosis (Yang et al. 2004), in medical planning (Abidi and Manickam 2002) and in knowledge modelling (Gardan and Gardan 2003). Finnie and Sun (2003) have proposed the new model of CBR process composed of the following main tasks: repartition, retrieval, reuse, revision and retaining, and applied it for case base building. Vong et al. (2002) have developed a CBR application to hydraulic circuit design for production machines. Li et al. (2002) have applied CBR in very new concept, agile fixture design. Mendes et al. (2003) have used case based reasoning in offshore petroleum well design, which acquires lot of experience by specialized engineers. Praehofer and Kerschbaummayr (1999) have applied CBR techniques to support the reusability of existing design artefacts in designing complex technical systems.

Several CBR systems have been built to support design, e.g. Cadet, which supports better conceptual design for electro mechanical devices (Sycara et al. 1992); Cadsyn, which provides guidance for architectural design and adapts existing designs for new buildings (Maher et al. 1995); Casecad, which use multimedia technology to store and present their cases to the user (Maher et al. 1995) and AskJef, which helps software engineers in designing human-machine interfaces (Barber et al. 1992).

4.1 CBR-based chemical process and equipment design

Even CBR has been used in engineering design quite extensively; its application to chemical engineering and process design has been limited.

Equipment design

CBR has been applied in mixing equipment selection and design (Kraslawski et al. 1995). Other applications were created for selection and design fluid mixing equipment and shell-and-tube heat exchangers (Koiranen and Hurme 1997) and solid-liquid separations (Virkki-Hatakka et al. 1997). Avramenko et al. (2004b, 2005) have developed CBR based design support system for selection internals for reactive distillation columns. The system can define the type and specification of geometric features of the internal devices of such a column.

Process design

Surma and Braunschweig (1996) have developed an application for retrieving most similar process flowsheets for hydrogenation C3 process. The application calculates the similarity of cases, i.e. flowsheets, as graphs. First the class of flowsheets is selected from the case base and the similarity between the flowsheet objects is calculated. After that the structural similarity is calculated. 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.

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 the index-based approach for evaluation of inherent safety. Using process characteristics as retrieval parameters, the nearest cases, where accidents or minor incidents have happened, are found from the database of good and bad designs. The found cases are scored to Safe Process Structure Subindex.

Arcos (2001) has developed a CBR application for aiding design and control of chemical adsorption plant. Case-base is composed of three different kinds of cases: performed installations, proposed installations, and pilot experiments. The case retrieval is two-stage process: First, minimum number of relevant cases is retrieved from the database.

Second, additional similarity criteria are used to ranking the retrieved cases. Adaptation phase is implemented by combining parts of solution of different cases, minimum and maximum values of parameters and equipment models. Pilot experiments are used to optimise the adaptation parameters.

Avramenko et al. (2004a) have developed a design methodology, which supports engineers in the conceptual design of wastewater treatment facilities and to help them to improve creativeness and effectiveness. The developed design tool is based on case-based reasoning and structural synthesis. The decision supporting system is composed of three databases (equipment, flowsheets, and methods) and two modules – (CBR system and conceptual design builder). If the CBR system could not find a suitable solution to the actual problem, the conceptual design builder generates a sequence of methods that are able to treat the wastewater of the given characteristics. The economic and efficiency evaluations are done based on data from the past application of the methods.

Separation process design

King et al. (1999) have applied CBR in the design of ternary azeotropic separation by using the residue curve maps approach. The cases stored on the case base include physical data (components, azeotropes, distillation boundaries and regions). Based on the description, the system is able to record several azeotropic distillation systems with two or three columns. If a similar case to a current problem exists, the system is able to give a qualitative description of the process.

Farkas et al. (2003) have developed a case-based library for distillation column and distillation sequences synthesis using MINLP. They have applied case-based design method for finding a proper MINLP model with superstructure and suggesting an initial point for performing design and optimisation of distillation system. After optimisation of selected MINLP model a solution of corresponding distillation synthesis problem can be obtained.

Control design

Xia et al. (1997) have built CBR based fault diagnosis and decision-making system for controlling pulp processes. CBR system is integrated with an information management system and distributed computer systems. This enables quick solution proposals in fault situations and the process is not dependent on operators' experience alone.

Roda et al. (1999) have applied CBR in process control of a biological wastewater treatment plant. In the process the inflow and the population of the micro organisms vary, the amount of detailed knowledge of the process is limited and only few online analysers are available. The CBR system informs the operations about the solution of the most alike problem in the past. Roda et al. (2001) have also developed similar CBR application for the supervision of a wastewater treatment plant, which has been successfully applied to a full-scale facility.

4.2 Separation process synthesis

A typical process designing task is to determine the configuration of a separation sequence. Several rule-based AI methods have been applied in separation process design (e.g. Barnicki and Fair 1990, 1992; Douglas 1995; Siirola 1996, Wahnshaff et. al 1993). It can be seen from the studies that the synthesis problem is difficult to handle by rules. In addition, creating rules (generalisations) causes information losses. Most of these methods are suitable only for limited types of separation processes.

Different methods for selecting the single separation and the separation sequence are listed below:

1. The use of an optimisation algorithm. For instance, a genetic optimisation algorithm is a feasible approach as shown by Hurme (1996). Another possible approach is MINLP, e.g. Novak et al. (1996).
2. The use of residue curve maps, e.g. Petlyuk (2004).
3. The use of knowledge-based / heuristic methods, e.g. thermally coupled distillation flowsheets, e.g. Rong et al. (2000).
4. The use of case-based reasoning. In this approach, there would be two levels of reasoning by CBR: The lower level, which concludes the separation method for single separations and the upper level which reasons on the sequence as discussed in this thesis.
5. Finding all possible separation combinations. This is feasible only in small cases. For example for four components and ten separation methods problem there are

5000 different sequences (Paper III). The combinatorial explosion takes place quickly when the number of products to be separated is increasing.

The objective of the following Chapter is to introduce a novel method for selecting feasible separation operations and process structures by case-based reasoning. This means finding most alike existing processes and applying the knowledge of their separation capacity and design for solving new problems in the early phases of process design. The method does not try to replace any rigorous simulations in the process design, but gives a few feasible ways to split the given feed into products. In this way, it limits the number of processes that need to be considered and gives a systematic way of utilising earlier designs in new problems.

4.3 CBR-based separation synthesis algorithm

Paper VI presents a new CBR-based separation process synthesis method. The main phases of the approach consist of 1) selection of the methods of single separations, 2) selection of separation sequences and 3) selection of combined (hybrid) separations. The phases of the algorithm are listed below and discussed in the following sections in more detail.

1. Selection of single separations
   a) Search method for the feasibility of conventional distillation based operations
   b) Search method for azeotropes (see subcase 1b); synthesis of azeotropic systems)
   c) Search method for suitable mass separation agents (MSA)
   d) Search method for other separation methods:
      i) Calculation of relative physical properties
      ii) Search method for separations based on feasible relative properties

1b) Selection of azeotropic separations
   a) Search method for separation in column in isobaric conditions
   b) Search method for separation in columns in non-isobaric conditions
   c) Separation by using MSA
   d) Separation by using MSA and non-isobaric pressure
   e) Separation by other means; reactive, membrane, extraction etc.

f) Separation by hybrid or combined operations

2. Separation sequencing by using as search criteria:
   - component names or types
   - relative volatilities of components
   - VF values of components (see Eq. 4.4)
   - coefficient of ease of separation values of components (Liu et al., 1987)

   And applying:

   a) Sequences in found cases or
   b) Sequence heuristics (if they are stored with cases)

3. Search for combined separation operations

   (See Section 4.8.2).

4.4 The selection of methods for single separation

Distillation is the most feasible way to separate components in the majority of cases. Therefore, the distillation related properties (e.g. relative volatilities) are studied first in the methodology (step 1a). The remaining separation problems are solved with further reasoning, which applies separation methods other than ordinary distillation. The main steps of the method discussed in Paper II are:

<u>Step 1a Feasibility of ordinary distillation:</u> Ordinary distillation is applied whenever the relative volatility (α) is large enough. The first search for the solution is made using component name, α's and reactivities as retrieval parameters. Relative volatilities are classified as easy ($\alpha \geq 1.2$), possible, where mass separating agent (MSA) could be useful ($1.1 < \alpha < 1.2$) and difficult ($\alpha \leq 1.1$). A more accurate search is made (capacity and component types as retrieval parameters) if several alternatives are found. If ordinary distillation is not feasible for all separations, continue to step 1b.

<u>Step 1b Identification of azeotropic distillation:</u> This is further discussed in Chapter 4.5.

<u>Step 1c Finding a suitable mass-separating agent (MSA):</u> A suitable mass-separating agent is searched for each binary component pair that cannot be separated by conventional distillation. The retrieval parameters used are e.g. component types, concentra-

tions, relative solubility parameter, dipole moment and dielectric constant. The found MSA is used for defining solubilities and other separation related properties for step 1d.

Step 1d Finding alternative separation methods: The principle is to apply separation method that utilises the largest property difference of the components to be separated. Relative physical property parameters are calculated for each component pair that can't be separated by ordinary distillation. The parameter values are compared to the feasibility limits of different separation methods (Jaksland et al., 1995, Qian and Lien 1994). The approach is used for finding the most important retrieval parameters.

In the next phase, other separation methods are searched using the relative parameters (min and max values) that are within the feasibility limits as retrieval parameters. For example, crystallisation is considered very feasible if the relative melting point is greater or equal to 1.2. In addition, a more detailed search (e.g. concentration, capacity and component types also as retrieval parameters) can be defined. If there are still several alternatives left, an economical comparison is needed.

The possibility of combined operations should be also checked. This is done in the last phase of the main algorithm.

4.4.1 Example on selecting separation methods for single separation

To present the principle of case-based process synthesis the separation of dimethylformamide (DMF), water and a light and a heavy boiling component is discussed in Paper III. The weight compositions and boiling points are given in Table 4.1. Synthesis of a separation process can be divided into subtasks of selection of single separations. In the following, the separation of DMF and water is discussed.

Table 4.1 Components in the case study

Component:	Amount	b.p.
Heavy	3 %	165 °C
DMF	9 %	153 °C
Water	83 %	100 °C
Light	5 %	25 °C

Query for specific cases

In a CBR system the user can make different types of queries in the database. The first query is made on DMF and water separation. As a result of this query, specific cases on distillation and extraction of these components are found (Figure 4.1).

	Attributes	Query (Solvent Recoveries)	14 Liquid-liquid extraction	16 Distillation
	Description	?	'DMF recovery'	'DMF recovery '
	Distillate HK	0.0005	0.0005	0.0005
	Feed HK	0.11	0.125	0.2
	Input Materials	'DMF, Water'	'DMF, Water	'DMF, Water
	Input Material Types	{Amines, Water}	{Amines, Water}	{Amines, Water}
	Mode	Continuous	Continuous	Continuous
>	Process Streams	?	?	?
	Quality Factor	?	?	?
	Separation Methods	?	{Extraction}	{Distillation}
v	Separations	?	Separation Structure	Separation Structure
v	Separation 1		Separation	Separation
v	Process Unit		Plate Column	Plate Column
>	Key Component - heavy		DMF	DMF
>	Key Component - light		Water	Water
	MSA		'chloroform'	?
	N(Real)		?	50.0
	Quality Factor		?	?
	Number of Cases found (max. 10): 10		Similarity: 0.955	Similarity: 0.95

Figure 4.1 Query and results on the case study

Creative queries

If new or more creative solutions are required, one can apply analogies or more general application cases in the CBR search. In this case a query can be made on separations for similar component types: Query for nearly similar boiling point can be defined as a boiling point interval (e.g. 150-160 °C). Query for similar polarity can be defined based on accentric factor. Relative properties can be calculated and search can be focused on those physical properties as shown by Paper 2. General search for different material types such as amines etc. can be selected for query. The material types available can be seen in Fig. 4 of Paper III.

General cases

General application cases are based on known guidelines. Paper III proposes that these cases can be represented in the same way as design cases in the case base. For instance, air stripping can be applied when $\gamma^{\infty}p > 35000$ kPa in 1000 ppm concentration range. The general application guidelines give a more complete but shallower coverage of the search space than specific cases as seen in Figure 3.2.

Negative cases

Negative cases can sometimes cancel the solutions proposed by general application guidelines. For instance, based on general application guidelines it might be possible to apply pervaporation for the separation but a negative case found in the database lists DMF as a component, which cannot be separated by pervaporation due to membrane problems. The current situation should be checked regularly due to technical development.

Adaptation

Since the cases found in the query (Figure 4.1) have different operating conditions (e.g. feed concentration), an adaptation of the case has to be done. For instance, a shortcut procedure to adapt distillation by using a separation factor S for different conditions has been given by Douglas et al. (1995).

$$S = \frac{y_L / y_H}{x_L / x_H} = \left(\frac{\overline{a}}{\sqrt{1 + D / Lz}} \right)^{hN_{real}} \tag{4.1}$$

Comparison

Comparison of the found cases can be done in principle by:

1) Costing, which requires dimensioning of equipment.
2) Shortcut comparisons. For instance, the method of Porter and Momoh (1991) uses column vapour flow for comparison. They have shown that the total vapour flow correlates well with total cost in distillation. This can be combined with the method of Sounders (1964) that allows economic comparison of three separation methods: normal and extractive distillation and extraction, based on the separation factor a.

4.5 The synthesis methods for azeotropic separations

The presence of azeotropes adds some difficulties to separations and the synthesis problem becomes much more complex. In general, to separate azeotropic mixtures various technologies may be used (Hilmen 2000):

1. Pressure-swing distillation with columns in different pressures are used to separate binary azeotropes, which change appreciably in composition over a moderate pres-

sure range or where a separating agent, which forms a pressure-sensitive azeotrope, is added to separate a pressure-insensitive azeotrope.

2. A third component can be added to modify the components´ relative volatility.
3. In heterogeneous azeotropic distillation added third component is partially miscible with one of the components.
4. Reactive distillation by the transformation of one of the components into a component, which does not form an azeotrope.
5. Salted distillation consists in adding an ionic salt that dissociates in the liquid mixture and changes the azeotrope composition.

The synthesis algorithm for azeotropic separations is a modification of the general synthesis algorithm in Section 4.5 (Paper V and VI). The steps for CBR searches are the following:

1. Separation in single or multiple columns in isobaric and non-isobaric pressure. Pressure changes can have a large effect on the vapour-liquid equilibrium compositions of azeotropic mixtures and thereby affect the possibilities to separate the mixture by ordinary distillation. By increasing or decreasing operating pressures in individual columns the distillation boundaries can be moved in the composition space or the azeotropes can even be made to appear or disappear.
2. Separation by using MSA (mass separating agent). MSA is searched for each binary component pair that cannot be separated by conventional distillation.
3. Separation by using MSA and non-isobaric pressure.
4. Separation by other means; reaction, membrane, extraction etc. The search is made for finding single separation method other than ordinary distillation to the azeotropic system.
5. Separation by hybrid or combined separations. Possibility of further combined or hybrid operations need also to be taken into account. After reasoning a feasible separation system, the user should consider combining the unit operations one by one as discussed in Section 4.6.2.

When azeotropes are present in the mixture, the definition of case description and retrieval parameters is more complex. One idea is to use the relative similarity based on the similarity of feed, product and azeotropic points as shown in Paper II. The retrieval parameters for a suitable MSA search are e.g. types of components to be separated, concentrations, relative solubility parameter, polarity and dielectric constant. The found MSA is used for defining solubilities and other separation related properties. If the MSA has not been used earlier for same components, studies that are more rigorous such as simulations and/or experiments, are needed to confirm the suitability. The approach can also be used for selection alternative mass separation agents as shown in Papers II and V.

4.6 Synthesis of separation sequence

The case-based reasoning approach can be used through an ‘upper level’ CBR for finding out a separation sequence. This is possible since the case base can also be used for storing feasible separation sequences in addition to information on single separations. The prototype case base was collected from the public literature. It includes less than one hundred separations and separation sequences, which allowed solving the case study problems presented. Simple column sequences for simple separations have also been generated and stored into the case base. Several feasible sequences, sometimes nearly equally good in the economic sense for the same problem, are stored into the case base. The search can be done (Paper VI):

1. Directly with *component names* or
2. *Component types* (e.g. aliphatic alcohol) or
3. In a more creative way by using analogies through *characteristic properties* of the components to be separated.

There are two alternative ways to interpret the search results:

i) Directly as feasible separation *sequences* or their sub sequences (Paper VI)
ii) As feasible separation *sequence heuristics*, which can to be applied on the design of the new sequence (Paper III).

In the first sequencing strategy it is possible to make searches by criteria, which are related to the separation properties of the component pairs as presented in Paper VI. The criteria should describe the difficulty of the separation by using properties such as boiling points, relative volatilities or coefficients of ease of separation (CES) (Liu et al., 1987). In the end the costs of the required separation tasks matter. Porter and Momoh

(1991) have suggested Eq. 4.2 as an approximate method of calculating the vapour flow V in a column, which can also serve as a simple estimate on the operating and capital costs:

$$V = D\left[1 + \frac{R_F}{(a-1)}\frac{F}{D}\right] \tag{4.2}$$

where

$$R_F = R/R_{\min} \tag{4.3}$$

The Equations 4.2 and 4.3 can be simplified to form a search criterion VF, which is calculated for all the component pairs to be separated. R_F was substituted with a typical value of 1.1.

$$\mathrm{VF} = (D + \frac{1.1F}{a-1})N \tag{4.4}$$

D and F are percentage concentrations of the component pair. N is the total number of components on the problem. It is used for scaling to make the values comparable between different separation problems.

If other methods than a conventional distillation is used, the values of relative volatilities are scaled to give a correct view of the economic feasibility. For extraction and extractive distillation the method of Sounders (1964) is employed for cost scaling. Other types of cost comparison charts are available elsewhere (Liu et al. 1987).

The method of finding separation sequences by CBR is the following: After the single separation methods are determined, the VF values are calculated for all component pairs to be separated by using percentage concentrations in the feed of the whole system. The VF is scaled with the number of components in the feed N to make the values comparable with problems of unequal number of components. After this, the search is made in the case base, which has known separation sequences stored with the component VF values. Since several sequences are often nearly as good at least in the theoretical sense (i.e. they give nearly similar values for the objective function) (Hurme 1996, Liu et al. 1987), it is useful to store several feasible sequences for one problem into the database.

It is also possible to split the problem into sub problems and search for these sub-sequences. In this case, a smaller part of the problem is searched from the database at a time.

The similarity can be calculated based on absolute or relative values of properties. For instance, the VF values can be scaled to unity for a certain base component to calculate relative similarities. For absolute similarities, there is no scaling. The similarity for the whole separation sequence is the average of the similarities of the single separations. The approach for separation sequence synthesis is demonstrated by the separation sequence problem presented in more detailed in Paper VI.

4.6.1 Example on separation sequence synthesis

Problem: Separate the mixture of light hydrocarbons shown in Table 4.2 into 'pure' components (Hartmann and Kaplick 1990).

Table 4.2 Problem feed compositions, adjacent relative volatilities, VF values and corresponding sequences found

	component	mol-%	α	VF	sequence	
1	Propane	13.7	2.53	224	y	u
2	i-Butane	11.7	1.26	588	y	u
3	n-butane	5.5	2.39	126	y	u, w
4	i-pentane	9.9	1.30	1000	x	u, v, w
5	n-pentane	26.4	2.16	400	x	v, w
6	i-hexane	5.6	1.31	854	x	v
7	n-hexane	27.2				

Solution: The values of search criterion VF are calculated for adjacent separations. A search is made among the case base sequences by trying to find similarity to any subset of query, which includes at least three separations.

The most similar subsequences found from the case base are shown in the Table 4 in Paper VI and marked with x and y in Table 4.3. The relative similarities are of 75% magnitude, which we have found generally acceptable.

The sequence synthesised based on the combination of the found two best cases (Hartmann and Kaplick 1990 and Smith 1995) is shown in Figure 4.2 left. The three lowest separations are from the first case (x) and the three uppermost from the latter case (y). Note that not all separations of the latter case (y) were used, but from the sequence the lightest component has been removed. This synthesis result corresponds to the optimum result reported (Hartmann and Kaplick 1990).

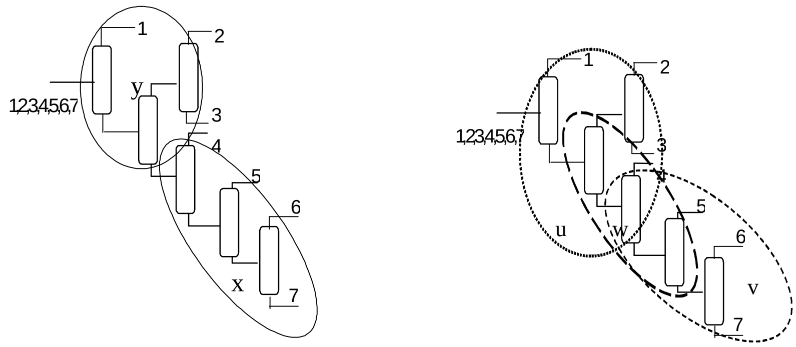

Figure 4.2 The synthesised separation sequences

The synthesised problem can also be solved by applying other cases found as shown in Figure 4.2 right. The sequences used now overlap and add more reliability to the result.

4.6.2 Combined operations

After the separation sequence synthesis the possibility of combined operations should be studied (Paper III). For example, a single column can separate several products using side streams. The approach for this is first to consider conventional separation sequences and then to try to combine single separations one by one. An alternative approach is to conclude possible combination operations from the retrieved cases as shown in Paper V Table 3.

Therefore, the approaches are:

1. Combine two sequential separations together
2. Search if analogous combined separation can be found from database by using relative volatilities etc.

Or

1. Calculate VF values of separations
2. Search if combined separation cases can be found in the database for those VF values.

4.7 CBR in process inherent safety design

The fundamental decisions in the conceptual design phase have a major effect on the inherent safety of process. Inherent safety is a principle, which emphasises the use of fundamentally safer principles in process designs. Thus, inherent safety is not based on added-on safety systems but on the safe fundamental properties of the process, such as safe chemicals, operating conditions and process systems used (Kletz 1998).

Experience based information on safety properties of existing process plants are available as industrial cases representing, which engineering solutions are preferable for certain purposes. Other sources of information are the accident reports and databases. They give information about the weaknesses of processes and operations. For the estimation of the inherent safety of the process configuration these information sources should be integrated into a case base

In the approach presented in Paper IV, the conventional process design is studied by CBR in different hierarchical levels (process, subprocess and equipment) to find out if known inherently safer solutions to the current process design problem exist. The found safer alternatives can then be substituted to the process concept and studied by simulation and pilot studies in more detail.

4.7.1 Application

Chemical processes have a very complex structure. The major problem in modelling such systems is the management of relationships between e.g. processes, equipment, components, and materials. Those relationships can be mostly modelled with object-oriented technique. Domain specific, complex data can be declared as data types of their own. This is benefit especially in conceptual process design, since the process structure is complicated and a flexible data structure is needed to represent the information.

The CBR retrieval phase of the application uses several distance functions. In the retrieval phase a set of retrieval parameter values of all cases (e.g. reactor type, relief system) in the case base are compared to the input data, which is defined by the user. The distance functions are closely presented in Paper IV (Sec. 2.1). The retrieval functions are quite simple, but the retrieval phase is diversified by focusing queries to different process levels. In addition, multiple database queries can be made in the case base.

4.7.2 Case study

An emulsion polymerisation system case study is given here to demonstrate, how the CBR method is used to improve the inherent safety of the process concept in an evolutionary manner by reasoning on several levels of detail.

A case base was formed of information based on the safety properties, accidents, design recommendations and existing designs of polymerisation processes. The information includes also general design recommendations of reactor systems.

4.7.3 Reasoning in different process levels

The process can be studied in various levels by altering the parameters and their weighting to find out which kinds of design cases (recommendations on good designs or warnings on bad case; e.g. accidents) are available to improve the design. In every level of reasoning, the found potentially safer solutions are used to substitute the features in existing design, which is improved gradually in an evolutionary way. The assessment, which design is better to another, can be based for instance to safety indices (Heikkilä et al. 1996) or user's own judgment. In addition, the textual case descriptions include qualitative evaluations on the safety features of designs found in the database.

First, the process was studied on a process or subprocess level to find out the main recommendations for the concept of this kind of system. As result cases containing recommendations of application of a semibatch principle to minimise the runaway hazard were found. On system level recommendations for the reactor and cooling system concept were searched for exothermic reactions, which possess fouling and viscous properties. The found cases can be adapted for reactor size, heat of reaction, heat capacity and heat transfer area to correspond the existing case. On equipment level, the possible relief equipment was studied using queries in the case base.

A quantitative verification that the improved process presented in Fig. 8 in Paper IV is better than the conventional batch process described in literature (Kroschwitz 1986) can be based on the calculation of Inherent Safety Index (Heikkilä et al. 1996) values of both processes. The conventional process has an index value of about 28-30 compared to the index value 16 of the improved process.

4.8 Process equipment selection and pre-design

Equipment design consists of equipment preliminary design, selection and detailed design. Selected equipment should be technically suitable, economic, reliable, easily maintain and safe to use. These considerations have to be taken into account, when computer-aided equipment design methodology is developed. In addition, design knowledge must be supported and maintained. Especially, the need of maintaining and updating the in-house knowledge is considerable.

Although, a design process of process equipment is often well known and precisely defined problem and rigours calculation methods are mature, the expertise knowledge is still needed. The knowledge consists of design algorithms and several heuristic rules, which are used by experts. The heuristic rules are based on previous design cases. The rules are generalizations of different cases, which always cause uncertainties.

The advantage of case-based reasoning in process equipment design is the possibility for direct using of exciting design cases. In addition, analogies based design can also be implemented by CBR technique. In the adaption phase, if the problem is well known and the calculation routines are exact, rigorous adaptation rules can be created.

4.8.1 Mixer selection and design

The basic idea of the prototype application presented in Paper I is to speed up the equipment design using existing design cases, and lists of equipment parts to make a set of practically sound designs. A possible set of designs is combined based on the information of the parts lists.

Standard design problems can be solved based on retrieval the nearest case; e.g. average bulk velocity and number of impellers. These solutions can be used as an excellent basis for more rigorous studies when the system does not behave ideally, since it cuts down the amount of be experiments needed. The new feature compared to the earlier study by Kraslawski et al. (1996) in the approach of Paper I is the use of combinatorial calculations in creating feasible combinations of mixer parts; the adaptation phase is implemented by using the combinatorial calculations and several process design equations.

The application includes the basic features of CBR technique and normal database functions like storing of cases etc. Exciting design cases consist of process and design parameters and equipment parts. The mixers are usually made by assembling from parts of several types and sizes, which can be combined in several feasible ways. To automate the selection of a feasible combination, all possible combinations are created in the application development phase. This is done beforehand, because even though several rules are applied to limit the combinations to feasible ones, the combinatorial explosion occurs very fast. The combination of equipment from its parts lists can be calculated from: (Paper I)

$$Y = X_1 \times X_2 \times X_3 \times \ldots \times X_N \tag{5.1}$$

where X vector consisting of equipment part lists

Y matrix consisting of equipment combined from its parts

The time-consuming combinatorial calculations need to be carried out only in the development phase and after each update of the equipment parts lists.

The basic steps of the system usage are: (Paper I)

- User defines the mixer problem
- The five nearest cases are retrieved, and user defines which case to adapt
- The mixing tank is adapted based on the selected case or defined by the user
- The criteria for suitable mixers is defined based on the data given by the user, data found in the nearest case and adaptation rules
- The suitable mixer(s) are selected from the feasible combinations and reported to the user

User defines the mixing problem by giving fluid volume, average bulk velocity in the tank, fluid viscosity and density and possibly tank dimensions. In the adaptation, e.g. number and type of impellers and the average bulk velocity are defined as the same as in the selected case. The mixing power is calculated based on these values, adapted tank dimensions and the user given fluid density and viscosity.

The values derived from the input, selected case and adaption calculations are combined as a report. The possible mixer combinations are selected based on this report. The criteria for suitable mixers are compiled and a list of possible mixers is created based on the required properties: (Paper I)

- the same impeller type as in the report
- equal impeller diameter as in the report
- shaft diameter is not less than the minimum shaft diameter in the report
- maximum impeller speed must be higher than required
- maximum power must be greater than the power required

If too many combinations are feasible, additional CBR system for selecting closest alternative to the case adapted may be needed or the search criteria need to be tightened.

4.8.2 Shell-and-tube heat exchanger pre-design

In Paper IV, a prototype application was developed to aid heat exchange equipment design. The program generates necessary input data including mechanical configuration for heat exchanger design simulators. In the heat exchanger application, the design quality is included. In this case, design quality is one evaluation parameter in the calculation of case similarity. In fact, design quality should be a combination of several parameters such as equipment safety, operational reliability, and economy. Quality parameters are also time dependent, which leads to following the lifetime of equipment in order to get a good case base.

The method presented is based on case-based reasoning (CBR) and an object database approach. The database contains collection design cases collected from open literature and existing process designs. The distance (or similarity) functions are same as used in inherent safe application (Paper IV).

The basic idea of the heat exchanger application is to use existing designs of heat exchangers for creating input parameters for heat exchanger design or dynamic process simulation programs. The most similar existing case is retrieved from the case base. Results from retrieval are necessary input data to dynamic process simulators, which require information on the type and mechanical dimensions of the heat exchangers to make a dynamic simulation in an early process design phase. In addition, a rigorous exchanger design, which is normally done by simulation programs such as HTRI or HTFS, can benefit from CBR by the reuse of design and operation information on the existing heat exchangers. Many aspects such as fouling and the feasible exchanger types are experience-based information. The detailed adaptation can be done using a heat exchanger simulator. Such simulator consists of necessary thermal design calculations for detailed heat exchanger design. The major benefit of CBR, when applied in the equipment design, is that it offers the experience of earlier designs needed in many engineering design tasks.

Input parameters of the heat exchanger model are in this case: fluid types, mass flows, operating pressures, possible phase changes, temperature differences between inflow and outflow and fluid temperatures of inflows etc. Output parameters define detailed fluid data, heat exchanger operating data, and heat exchanger mechanical design data including design quality. Retrieval calculations are constructed as described above.

Results from retrieval are the TEMA type for heat exchangers, position (vertica1/horizontal), shells per unit, number of units, and number of passes. The TEMA type defines front-end head types, rear end head types, and shell types of shell-and-tube heat exchangers.

4.9 The pros and cons of case-based reasoning in process design and equipment pre-design

CBR combines the traditional engineering experience-based methods with computer based design support systems, which enable the reuse of exiting design information. The systematic use of existing information and the feed back of the successful existing designs is a method of continuous improvement of engineering work in companies as presented in Paper III.

The CBR approach is beneficial when the problems are not completely understood so that an exact model cannot be built but experimental work, pilot studies etc. are required. The problem does not need to be completely defined before starting to reason about possible solutions. Implementation of the method is reduced to identifying significant features that describe the case, which is an easier task than creating an explicit model. In addition, failed experiences can be included in the case base to allow learning from earlier failures. CBR proposes solutions quickly, in this way fastening, and directing 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. Therefore, there should be a possibility to use search criteria in a creative way. This is presented in Paper II by using search by analogies. Case adaptation is needed to transform the retrieved cases to correspond to the problem.

Because generalisations are not needed in CBR, no data is lost. CBR gives answers to design problems in a straightforward way. The results are dependent on the retrieval parameters and the adaptation applied. The strong interaction with the user makes the flexible and interactive use of existing data and design experience possible. The CBR search can be focused on different aspects by defining new search criteria and weighting retrieval criteria differently. In this way, the same case base can be used for several types of tasks. The system learns by updating the information of the database allowing continuous learning.

In order to use CBR, the existing designs need to be systematically stored in a case base together with an estimate of the quality of the design (Koiranen and Hurme, 1997). This approach offers also an efficient tool for documentation of design activities. In this way, the operation experience from the designs is stored for further use. All this forms an organised institutional memory of the company, which also includes the experience of the senior process designers presented as design cases. This is a clear improvement to the typical existing situation, where the information is difficult to reuse because of unsystematic documentation and filing practice.

One of the most important points to be considered is the definition of quality factors as presented in Paper III. These factors describe the value and reliability of a design case. The quality of the solution found and applied to the current problem depends on the quality of the solutions stored in the case base and the validity of the adaptation rules employed in the reasoning. Two factors are used: technical maturity and performance (goodness) factor as presented in Table 4.3. 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 even better result but involves a larger risk.

Table 4.3 Technical maturity and performance factor (Paper III)

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)

A disadvantage of case-based reasoning is that users might rely on previous experience without validating it in the new situation. Users might allow cases to bias new problem solutions. In addition, when users are doing reasoning, they might not recall all appropriate sets of cases for solving problems. (Kolodner 1993)

The case base must cover the majority of the problem domain, or the system will run into problems when cases that have no real match in the case base appears, since no solution can be proposed. Adding new cases will not necessarily make a system converge towards greater reliability, as cases add only local improvement. The case base should also have sufficiently similar cases otherwise the retrieved solution may be inappropriate.

Adaptation is still a big research issue in case-based reasoning that is also getting increasingly important in practice as the complexity of applications increases. Despite several workshops and published papers that try to systematically analyse the different approaches to adaptation, general or systematic approaches for implementing the adaptation module of a CBR system are still missing.

5. INFORMATION MANAGEMENT DURING PROCESS LIFE CYCLE

5.1 Introduction

Typical process lifecycle steps include: development, conceptual design, detailed design, procurement and installation, construction, start-up, operation, retrofit and commissioning. All of these steps produce different kind of information of the process, which is needed later. In addition, the background information and work processes, such as why certain decision is made, are information produced, but not recorded by the existing practice. Part of the recorded information is also lost because of the documents do not always follow the delivery of the process or they are not updated later.

Commonly, information management between interest groups during an engineering project is based on exchange of documents. Engineering and other information systems are integrated by exchanging either physical documents or electrical documents of some form. Different companies commonly have their own data models. Information must be transferred to a form that is conformant with another data model used by another company. When the number of collaborating companies increases, this approach becomes laborious and thus expensive.

An improvement of this is a lifecycle-oriented perspective to information management, which emphasizes an integrated consideration of data (such as flowsheets, simulation models, equipment data, etc.) and work processes. As opposed to a data-centric view, not only the most recent state of the data is made available but also a comprehensible representation of its evolution, namely the work processes conducted to transform the data from one state into another together with the decision-making processes. (Bayer and Marquardt, 2004)

The information management is started in the conceptual design, when the data structures are generated. The logical concepts identified during conceptual modelling need to be formalized to a general data model. This data model should not only serve for the implementation of specific process models in a model library but also for the representation of knowledge about models and the modelling process involved.

The study presented in this Chapter is focused on the lifecycle information management in the conceptual design phase.

5.2 Information management systems in chemical engineering

In recent years, numerous approaches have been developed to support the activities in chemical process design. In following, few systems are presented.

Marquardt and Nagl (2004) have studied the early phases of the chemical process design lifecycle, the conceptual design and front-end engineering. The research issues were development of an integrated information model of the design process, a number of innovative functionalities to support collaborative design, and a-posterior integration of existing software tools to an integrated design support environment.

Open issues of information modelling are also discussed by Schneider and Marquardt (2002), and Bayer and Marquardt (2004). They have developed a conceptual model framework CliP, which holds solution approaches for the integrated representation of information and work processes, the description of documents as carriers of data, and the integration of existing data models. CliP can also serve as an integration basis for existing information models.

The design process management system AHEAD (Heller et al. 2004) is designed specifically for dynamic design processes. AHEAD also supports the management of inter-organizational design processes. For example, a sub process may be delegated to a contractor, which receives information only about those parts of the overall process that are relevant for the contract.

N-dim (Subrahmanian et al. 1997, Westerberg et al. 1997) is a design process support system that strives to support engineering design and also management of the design process. It can be used to store formal and informal information collected during the entire life cycle of an engineering project.

KBDS (Bañares-Alcàntara 1995, Bañares-Alcàntara and Lababidi, 1995) supports the design process by recording design alternatives, which are related to design objectives.

Process support is integrated into a flow sheet tool, which represents design alternatives and their rationales. This approach has been developed further in PRIME (Pohl et al. 1999) and MODKIT (Bogusch et al. 2001), each of which relies on a process engine for providing both process guidance and process automation at pre-defined communication and synchronization points. MODKIT supports tasks like the graphical definition of the structure, the behavioural description, and the documentation of a process model in a work process oriented manner. Within MODKIT, code for different simulators can be generated, leading to a modelling process, which is independent from a specific simulator.

One approach to manage design processes is the web-service framework (Kondelin et al. 2004). A common framework specification have been defined for process plant information management in order to support different phases of plant life cycle and open extensibility for value-added services in a distributed working environment consisting of different companies.

Paper VII presents a new web-service based approach in conceptual process design; parameterised constructors, which are able to construct process and produce initial data for control system configuration. Constructors use unit process or larger sub-process templates, which consist of upper level process structures, control loop descriptions and detailed process structures. Unit processes and equipment models are defined to the plant model library and based on the user selections the plant model is dynamically created by the constructors. The constructors also generate control scheme.

5.3 A web service based framework

In order to achieve tool integration for the whole life cycle of a process plant, a domain specific framework specification is needed. The specification should take into account the software architectural aspects and the variety of existing production related information systems that end users have. (Paper VII)

Compared to the use of separate systems, the proposed service framework provides

- a common user interface and knowledge presentation
- a common way to extend the existing systems with new value-added services

The framework can be divided into core services, framework services and value added services. The core services represent legacy systems in the architecture such as process design systems, simulators or control systems (Kondelin et al. 2004). The most important core service from the viewpoint of conceptual design is the plant model core service. The plant model service will contain information that is accumulated in design time, updated and specified in operational phase, and used by various services of the framework during various life cycle phases.

5.3.1 Data model

In different phases of the life cycle, several interest groups interact and need to exchange information between each other. Especially in the early stages of the process life cycle a lot of information is case sensitive. Knowledge and information management becomes an important issue, which has to rely on data models.

There exist several different data-centric standardisation efforts or an information exchange standard e.g. international: ISO 15926 (ISO 15926-1 2004), STEP (ISO10303-221 2005, ISO10303-227 2005), AEX (FIATECH 2005) and national: PSK XML (PSK 2005) data transfer model. Recently, the data model research has been focused on the semantic web, which provided a framework for data sharing among application, enterprise and community boundaries.

A common data model offers possibility for data transformations between different application software attached to the framework. For example, different management, design and simulation tools are used at different stages of the process life cycle and many of them are incompatible.

5.3.2 Global CAPE-OPEN

Global CAPE-OPEN is a project for standardising communication between components in process engineering, leading to the availability of software components offered by vendors, research institutes and specialised suppliers. This will enable the process industries to reach new quality and productivity levels in designing and operating their plants (CO-LaN, 2005).

The scope of Global CAPE-OPEN is extended to cover other areas related to process simulation as well. This comprises primarily set up and configuration support for component-based simulation environments, as well as an export format for declaratively specified process models.

5.4 Web-service based approach in conceptual design

Automatic supporting of conceptual design means creating a system that takes the limited information available early in a project and maps it into a model of the result at the desired accuracy. To make this feasible requires simplification by eliminating all non-essential details.

Open extensibility for value-added services is becoming an essential issue in information management during all phases of process life cycle, from process design to demolition. The progress in information technologies offers possibilities for new kind of integration of process design systems, simulation tools and different value-added services such as dimensioning tools and intelligent constructors introduced in Paper VII. The new value-added services are implemented as web services. A common data model, manipulated through web service interfaces, links and reflects the different requirements of the process and automation design, delivery project and plant operation and maintenance.

5.4.1 The plant model

The plant model is actually a domain specific meta-model that describes how object types are defined. Object types are created by defining plant object types, property types, and relation types according to the meta-model. In addition, relation rules that restrict relations between objects and properties are defined. Object types describe the common taxonomy for plant object instances. In the framework, instances are represented and transferred as XML fragments that conform to the plant data model, which is defined by utilizing XML Schema type definitions (Kondelin et. al., 2004).

As described in Paper VII, there are four different object types (Fig. 5.1): The conceptual function type represents upper level functions of some kind, such as pressure change. The constructional function type represents more specific functions analogous with objects in a PI-diagram. The product type defines generic product in the plant, not containing information of the individual physical objects. The product type realizes the functionality of the constructional function type i.e. an equipment type. The individual type defines physical object in the plant, containing information such as serial number, maintenance history etc.

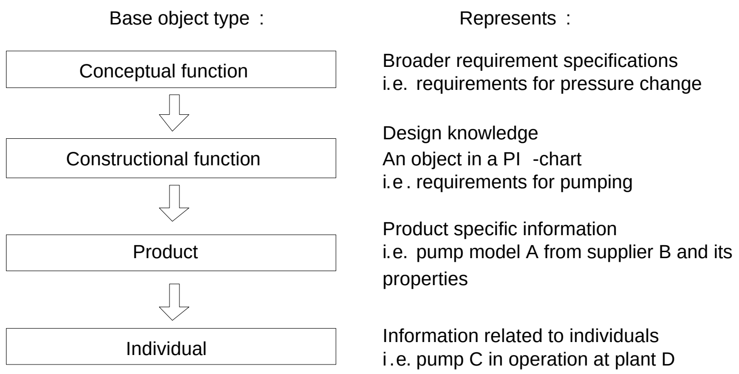

Figure 5.1 Base object types.

5.4.2 A value added service: Parameterised constructors

Parameterised constructors can be applied to construct process and produce initial data for configuration. They use unit process templates and larger sub-process readily available in a plant model library. The templates consist of upper level process structures, control descriptions and detailed process structures. Parameterised constructors are used to: (Paper VII)

- Generate ’automatically’ structures of processes and/or parts of the processes.
- Intensify routine process design tasks.
- Generate operational descriptions. Based on the loop type descriptions detailed initial data is generated for control engineers for design purposes, operation information for operators is also given.
- Integrate operability and flexibility considerations into the process synthesis procedures.

The benefit of using constructors is that the preliminary process design can be at first defined in a more general level. As the design proceeds, more accurate models (e.g. PI and automation diagrams, simulation models) are used. Unit processes and equipment models are defined to the plant model library and based on the user selections the plant model is dynamically created. The constructors also generate control scheme according to the user's selections and include it into the plant model. As a result, detailed operational descriptions are generated and are readily available to the control system supplier for configuration.

The use of constructors can also be included in optimisation problems. For instance, the selection of template models can be described as binary variables as in MINLP optimisation. In this approach, the optimiser selects the parameters and the constructors create the plant model used for the cost function evaluation based on the parameters. If the resulting model is simple enough, as it should be in the first flowsheet models, the calculation speed is not a problem with wisely chosen cost function and optimisation algorithm.

5.4.3 Process templates

Similar process structures are often used in the design of processes. Defining templates for the common sub process structures intensifies routine process design tasks. Such typical sub processes in the pulp and paper plants are e.g. a pulper, disc filter, pulp tower and a proportioner. Existing design knowledge, like upper level process structures, automation diagrams and detailed process structures, is stored in the templates as shown in Paper VII.

5.5 Case study: Design a new fibre refining process

In Paper VII, parameterised constructors and templates were created for a fibre line process in paper industry to be used in an engineering company. Designing a new fibre refining process for paper machine is given as a case study. The initial data and parameters for the conceptual model are derived from basis of design i.e. requirement specifications (raw materials, products, capacity, consistency, specific refining energy, etc.).

The unit process templates, from which the process is composed, are chosen by the designer. Depending on user's input and selections, the conceptual model is further composed to the constructional plant model by the constructors.

Operational description definitions i.e. loop type description of commonly used control systems are readily defined in the standard loop model library. The user selects and checks initial information for the control system design, e.g. which kind of control structures is used. The constructor ensures that the operational description e.g. of liquid level control of the pulp tower is transformed to an automation schema.

When the constructional plant model is defined, the user can transform data from the plant model to simulation service, where equipment selections and dimensioning, different operation value studies and mass and energy balance calculations are made.

Preliminary process design is the most essential and decisive prerequisite for control system provider selection and system design. It reduces iterations and eliminates problems resulting from insufficient or incorrect information. Efficient utilisation of the simulation and the parameterised constructor services can reduce iterations and shorten the total design process.

The control system application design is based on operational descriptions and control and interlocking diagrams. The operational descriptions are selected or created during the preliminary unit process design by using the constructor service and standard loop model library. Iterations and mutual checks between the process and the control system design will be eliminated or at least minimised. In addition, control system hardware and application design can be designed concurrently.

The control system application designer gets operational descriptions, diagrams and control loop specific information, view specifications etc. from the plant model database and transforms these general descriptions to system specific. The result includes applications and configurations, user interface and views, external interfaces etc. which are saved to the plant model database.

6. FUTURE ASPECTS IN PROCESS DESIGN

Future growth within the chemical process industries is likely to involve even keener competition with greater impact from factors such as raw material and energy availability, climate change mitigation, sustainability, and inherent safety. The future of process design has the following trends: 1) Increasing productivity and selectivity through intensification of operations; 2) Designing novel equipment based on scientific principles and new production methods using a multiscale approach to process modelling and control; 3) Implementing multiscale application of computational chemical engineering modelling and simulation to real-life situations from the molecular scale to the production scale; 4) Extending process design methodology: new algorithms for process synthesis, new design strategies, and new computerized implementations. Future process synthesis methods are also likely to involve with other parts of the process design including in particular process and catalytic chemistry and operability and control expertise. (Barnicki and Siirola 2004), (Charpentier 2003)

On the other hand, information technology has been becoming increasingly important in all areas of engineering during the last few years. Much of the progress achieved in chemical engineering would not have been possible without the enabling methods and tools provided by information technology. This trend will continue in the future but most likely with a considerably wider scope. While individual software tools and services have been in focus until recently, their integration into engineering work processes is an emerging and challenging area of research and development.

The industry is moving towards a widespread strategic use of information technology to better perform their business processes in research and development, in process design as well as in procurement, manufacturing, and distribution. The vendor companies are exploring this business opportunity and serving the needs of their customers. The most important drawback of the software engineering approaches is still the missing domain specific knowledge, which is required to effectively represent design processes in chemical engineering. Another drawback is that the market in number copies of conceptual design automation systems is significantly smaller than the market for detail design systems where every engineer may be a user. To be effective, conceptual design tools have to incorporate significant design knowledge. On the other hand, conceptual design automation solutions are business tools that may have remarkable business impact.

Information technology standards will gain increasing attention. The standardization process is tedious for technical, organizational and economical reasons. The operating companies have to drive that process because it is primarily in their interest and to a lesser extent in the interest of software vendors. Non-profit institutions (e.g. PSK-Standardization in Finland) have been formed to manage and facilitate the standardization process, maintain existing standards, support software developers in implementing and testing the standards and finally certify compliance of software with the standard.

One potential solution for information management during plant lifecycle could be the web-service framework, which is presently being developed in VTT Industrial Systems (Kondelin et al. 2004). A standardized semantic data model i.e. a plant model is the base for intelligent application services, which support e.g. decision making, process and control system design and layout design tasks. In addition, simulation models (i.e. steady-state models, dynamic large scale process models, CFD models) can be integrated into this information management environment. Models can be instantiated with data from the plant model and simulation results can be transferred back the plant model. The integration of simulation models can be implemented as component based that is different users are able to aggregate the simulation model just from needed parts. In the design phase, the standardized plant model data can be created and analyzed using different value added services e.g. parameterized constructors (see Chap. 5.), equipment selection tools and interfering tools for operation and maintenance.

As conceptual plant modelling techniques develops there is an opportunity for simulation and plant modelling integration. This means that simulation would not be a separate discipline anymore but an integrated part of other information management in plant delivery project. Based on standardisation efforts described before an open source platform should be implemented for distributed ’virtual plant design’ environment. The business would no longer be in simulator platform licenses but in plant model configurations and simulation components that can be run as part of plant model run times.

7. CONCLUSIONS AND DISCUSSION

The main target of this thesis is to study and present methods how to intensify the conceptual process design phase. The developed methods and tools are applied to separation process synthesis, process equipment selection and pre-design, and process design support systems.

The object of computer-aided design is better control of design knowledge; speeding up design by defining in the early phases the design alternatives to be studied further by rigorous methods. Systematic documentation of design projects is also essential. The major design decisions have to be made as early as possible in the process design.

In this thesis, case-based reasoning technique has been applied successfully in conceptual process and equipment design. The main benefit of CBR application is that readily available existing knowledge can be utilised systematically also in very large and complex problems like process synthesis and design. In this way the time-consuming conceptual screening phase in a design project can be fastened. Because generalisations are not needed in CBR, no data is lost. CBR gives answers for design problems in a straightforward way, but the results are dependent on the retrieval parameters and the adaptation applied. The strong interaction with the user makes the flexible and interactive use of existing data and design experience possible. The retrieval can be focused on different aspects by defining new search criteria and in this way the same case base can be used for several types of tasks.

The system learns by updating the information in the case base. In fact, the system can function as an institutional memory and therefore the use of CBR can enhance a systematic documentation practice in the company. Because of its principle, CBR applications are limited to the use of existing knowledge, but creativity can be introduced to by using analogies.

In this thesis, new approach, case-based reasoning for separation process synthesis is presented. The CBR method is based on three phases: 1) selection of the methods of single separations; 2) selection of separation sequences; and 3) selection of combined (hybrid) separations. With this method, selection of separation process alternatives is directed in feasible solutions and in this way the conceptual design process is fastened. The advantage compared to rule-based methods is that all the existing knowledge is available as cases and can be utilised in a non-reduced form. The method is also very flexible because the user can focus the search by defining more accurate search parameters if several nearly similar solution possibilities are available.

The mixer and heat exchanger applications have been developed on Paper I and IV to illustrate the possibilities of CBR in process equipment pre-design. Although the applications are prototypes, the methodology itself is fully applicable and the equipment manufacturers and suppliers can benefit from time savings, increased robustness in design and intensified design work routine.

Object-oriented approach and object database techniques allow more flexible application development especially in complex process design cases. Object database combines the semantic of object-oriented approach with data management and query facilities of a database system. The inherent safety application presented was probably the first in chemical engineering domain, where have been used CBR and object database technique were used together.

A common framework specification for process plant information management, web-service framework, has been shortly presented. The web-service framework supports different phases of plant life cycle and open extensibility for value-added services in a distributed working environment consisting of different companies. A web-service based approach in conceptual process design, parameterised constructors, which are able to construct process and initial data for control system configuration is introduced. The benefit of using constructors is that the preliminary process design task can be started in a more general level. As the design work proceeds, more accurate models (e.g. PID and automation diagrams, simulation models) can be used. Unit processes and equipment models are readily defined in the plant model library and based on the user selections the plant model is simultaneously created. The constructors can also generate control scheme according to the user’s selections and include it into the plant model.

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