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Conflict-based Method for Conceptual Process Synthesis

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ABSTRACT

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The changing business environment demands that chemical industrial processes be designed such that they enable the attainment of multi-objective requirements and the enhancement of innovative design activities. The requirements and key issues for conceptual process synthesis have changed and are no longer those of conventional process design; there is an increased emphasis on innovative research to develop new concepts, novel techniques and processes. A central issue, how to enhance the creativity of the design process, requires further research into methodologies.

The thesis presents a conflict-based methodology for conceptual process synthesis. The motivation of the work is to support decision-making in design and synthesis and to enhance the creativity of design activities. It deals with the multi-objective requirements and combinatorially complex nature of process synthesis. The work is carried out based on a new concept and design paradigm adapted from Theory of Inventive Problem Solving methodology (TRIZ). TRIZ is claimed to be a 'systematic creativity' framework thanks to its knowledge based and evolutionary-directed nature. The conflict concept, when applied to process synthesis, throws new lights on design problems and activities. The conflict model is proposed as a way of describing design problems and handling design information. The design tasks are represented as groups of conflicts and conflict table is built as the design tool. The general design paradigm is formulated to handle conflicts in both the early and detailed design stages.

The methodology developed reflects the conflict nature of process design and synthesis. The method is implemented and verified through case studies of distillation system design, reactor/separator network design and waste minimization. Handling the various levels of conflicts evolve possible design alternatives in a systematic procedure which consists of establishing an efficient and compact solution space for the detailed design stage. The approach also provides the information to bridge the gap between the application of qualitative knowledge in the early stage and quantitative techniques in the detailed design stage. Enhancement of creativity is realized through the better understanding of the design problems gained from the conflict concept and in the improvement in engineering design practice via the systematic nature of the approach.

Keywords: Conflict-based method; Methodology; Creativity; TRIZ; Conceptual process synthesis; Multi-objective; Distillation; Reactor/separator; Waste minimization

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FOREWORD

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Lappeenranta, July 2004

Xiaoning Li

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LIST OF PUBLICATIONS

The thesis includes the following original publications which are referred to in the text by their assigned Roman numbers corresponds to the Appendix (**IV – IX**)

IV. Li, X. N., Rong, B. G., and Kraslawski, A., (2002), *Synthesis of Reactor/Separator Networks by the Conflict-based Analysis Approach*, 12th European Symposium on Computer Aided Process Engineering, Computer-Aided Chemical Engineering, **10**, 241-246, Elsevier.

V. Li, X. N., Rong, B. G., and Kraslawski, A., (2001), *TRIZ-Based Creative Retrofitting of Complex Distillation Processes-An Industrial Case Study*, 11th European Symposium on Computer Aided Process Engineering, Computer-Aided Chemical Engineering, **9**, 439-444, Elsevier.

VI. Li, X. N., Rong, B. G., Kraslawski, A., and Nyström, L., (2003), *A Conflict-based Approach for Process Synthesis with Waste Minimization*, 13th European Symposium on Computer Aided Process Engineering, Computer-Aided Chemical Engineering, **14**, 209 -214, Elsevier.

VII. Li, X. N., Lahdenperä, E., Rong, B. G., and Kraslawski, A., (2003), *Multi-objective Process Optimization by Applying Conflict-based Approach,* Proceedings of the Fourth International Conference on Foundations of Computer-Aided Process Operations, 623-626, CACHE Corp.

VIII. Li, X. N., Lahdenperä, E., Rong, B. G., Kraslawski, A., Nyström, L., (2003), *Conflict-based Approach for Multi-objective Synthesis of Reactor/Separator System,* 8th International Symposium on Process System Engineering, Computer-Aided Chemical Engineering, **15B**, 946-956, Elsevier.

IX. Li, X. N., Kraslawski, A., (2004), *Conceptual Process Synthesis: Past and Current Trends*, special issue of Chemical Engineering and Processing, **43**, No.5, 589-600.

Associated Publications

Parts of the results that are introduced here have been published in associated publications. The following publications are not included in this thesis.

Li, X. N., Rong, B. G., and Kraslawski, A., (2001), *TRIZ-Tools for Creativity Support in Chemical Process Design*, 6th World Congress of Chemical Engineering, Sep 23-27, Australia.

Lahdenperä, E., Li, X. N., (2003) *A Cluster Computing Approach Using Parallel Simulated Annealing for Multi-objective Process Optimization,* Proceedings of 8th International Symposium on Process System Engineering, Computer-Aided Chemical Engineering, **15B**, 1295 - 1304, Elsevier.

Li, X. N., Kraslawski, A., (2004), *Conflict-based Method for Process Synthesis,* Proceedings of the Sixth International Conference of Computer Aided Process Design, 291-294, CACHE Corp.

The Author’s Contribution in the Appended Publications

IV. The author developed the research concept. She implemented the case study and wrote the manuscript together with co-authors.

V. The author carried out the case study. She planned design procedure and performed all necessary calculations. The paper is written by the author together with co-authors.

VI. The author carried out the case study. She developed the research concept and wrote the paper based on the obtained results.

VII. The author created the design and simulation procedure. The programme was made together with the co-authors. She carried out all calculations and wrote the paper together with co-authors.

VIII. The author developed the research concept. She performed all the calculations and interpreted obtained results. The paper is written by the author together with co-authors

IX. The author made the literature survey. She summarized the research topics and wrote the paper together with co-author.

1 INTRODUCTION

1.1 Subject of Thesis

In the past decade, the chemical industry has experienced a rapidly changing environment. With the more demanding business environment, the industrial processes have to be designed and operated in a way to enable the fulfilment of multi-objective requirements and enhancement of innovative design activities. Consequently, the requirements and issues for conceptual process design have changed and no longer follow conventional process design. This has led to growing interest in creativity enhancement and innovative research in process design compared to incremental improvements in existing processes. The important stage of design where the role of creativity support is of crucial importance is the phase of conceptual synthesis. Therefore the important practical and theoretical issue, how to enhance creativity in conceptual process design, requires further studies into applicable design methodologies.

A design methodology is an attempt to systematize design activities, in this case conceptual process synthesis. Process synthesis is a part of the overall chemical innovation process which leads from the identification of a need to the construction and operation of a facility to produce materials believed to satisfy that need (Siirola, 1996). A good process design methodology should not only provide solution scope, as it does in the traditional sense, but also show the way to creative solutions (Tanskanen, Ph.D thesis, 1999). The term ‘systematic creativity’ describes the tendency of developing a design methodology towards a way of enhancing the creativity of the design activities. It means that the purpose of the design method is to make the problem solving process progress from the random to the systematic while keeping and exploring all possibilities of good solutions (Mann and Dewulf, 2002). Therefore special attention must be paid to the issue of the development of a method ensuring ‘systematic creativity’ in design which allows for the conscious and systematic creation of highly innovative designs.

The thesis presents a methodology for conceptual process synthesis. The motivation of the work is to support the decision-making of design and synthesis and to enhance the creativity of design activities. The thesis deals with the multi-objective requirements and combinatorially complex nature of process synthesis. It also provides the overall context of process synthesis to assist the search for optimal solutions. It is claimed that the concepts and activities of process synthesis can be modelled and creativity can be simultaneously supported using the developed methodology.

1.2 Overview of Thesis

The main research issues raised in this thesis are:

- *How to model information handling for design knowledge based on the new design concept*
- *How to model the design activities*
- *What are the problem solving strategies*

Answers to these questions are explored with the development of a methodology which involves the steps below:

1. Understand the problems and formulate the basic issues.

Here the problem is multi-objective synthesis of chemical processes. Section 2 gives an overview of process synthesis, the existing design methods and their applications. Section 3 gives a definition of creativity in design and the modes of enhancing creativity for design. TRIZ methodology (Theory of Inventive Problem Solving), the method utilized in this work, is introduced and its characteristics are discussed.

2. Characterize the process synthesis via the new concept.

Section 4 presents a definition of process synthesis based on the new concept. It interprets the conceptual model for design problem presentation and for information handling of design knowledge. The classes of design problem are formulated into conflicts among the design objectives and process characteristics.

3. Formulate the design paradigm.

Section 4 shows the formulated general paradigm for conceptual process synthesis at both early and detailed design stages. The design procedure combines the conflict-based method with a quantitative technique, simulation based optimization. The strategies of guiding decision making are explored for the application of the developed method.

4. Develop the design tools.

Section 4 presents the way of building design tools, the conflict table (or contradiction matrix), to support conceptual process synthesis. The process is illustrated by building the conflict table for a reactor/separator system.

5. Implement the design methodology via the case studies.

Section 5 presents applications to illustrate the developed methodology. The applications deal with hierarchical decisions and multiple conflicting goals. Three examples of process synthesis have been studied; distillation system design, reactor/separator network design, and waste minimization design. Through the case studies, Section 5 also presents the proposed design paradigm which deals with conflicts in the context of the whole design process. The conflict-based analysis provides information to bridge the gap between the application of qualitative knowledge in the early design stage and the quantitative techniques of the detailed design stage.

6. Summary

Section 6 draws together the conclusions of this work and reviews the main contributions of the thesis. The section ends with discussion and perspectives for future work.

2 CONCEPTUAL PROCESS SYNTHESIS

2.1 Process Design

Process design is a complex problem solving activity. It begins with an acknowledgment of needs and dissatisfaction with the current state of affairs, and realization that some action must take place in order to solve the problem (Braha and Maimon, 1998). The definition of engineering design by Dym and Levitt (Dym, 1995) is: Design is the systematic, intelligent generation and evaluation of specifications for artefacts whose form and function achieve stated objectives and satisfy specified constraints.

The major features of a design problem are its under-defined, open-ended nature and the requirement of the satisfaction of multiple criteria; while only a very small fraction of the information needed to solve a design problem is available at the stage of its formulation. More and more information becomes available during the process of solving a design problem. Design is difficult because there exists a large number (10^4 to 10^9) of ways to accomplish the same design goal (Douglas, 1988). Moreover, with the more demanding business environment, the chemical processes have to be designed and operated in a way enabling the simultaneous fulfilment of economic criteria, safety and environmental requirements as well as other objectives. Usually, optimum decisions will not be sought and satisfactory decisions are finally accepted by the designers. The difficulties of solving design problems determine that design is a stepwise, iterative, and evolutionary transformation process (Braha and Maimon, 1998).

French (1985) has developed a general model of the design process, shown in Figure 1. It is one of the most widely cited models of the design process. The circles represent the evolution stages of the design. The rectangles indicate the steps of the design activities. As the figure shows, the design process starts with a stated need, then through a process of analysing the problems and gathering relevant data, the design process arrives

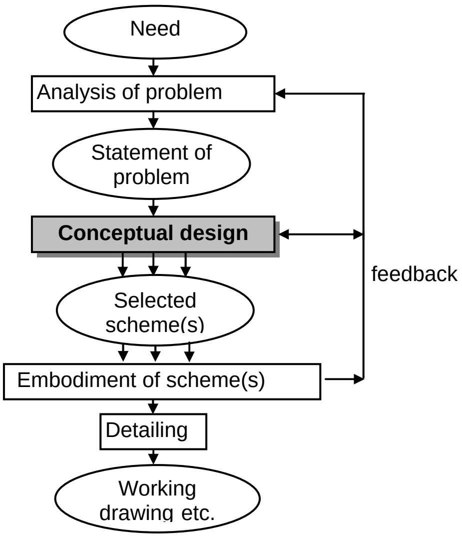


Fig. 1. French’s model of the design process

at a clear statement of the problem. Then starts the conceptual design stage, when the search begins for design schemes to solve the formulated design problem. The detailed design consists of the selection of the optimal solutions from among the proposed schemes obtained in the conceptual design phase. The conceptual design stage is a high-level decision making process and the most open-ended part of the design process. In this work, the main emphasis is on conceptual process synthesis.

2.2 Conceptual Process Synthesis (CPS)

Conceptual process synthesis (CPS) is becoming an increasingly important field of activity in industry and academia. According to Harmsen (1999), the total cost savings by industrial application of process synthesis range from 20 to 60%. During the last decades, process synthesis has experienced significant changes with respect to research issues as well as to application domains. Its development is based on the need to satisfy external requirements (economic, social, environmental etc.) and implement new technological concepts.

Amundson’s report (1988) gave a well-structured and still current picture of CPS. According to this report, there are three scales of CPS development: the micro, meso and macro scale. The picture of CPS development extends to the detailed issues based on the review work done by Li et al. (2004) as shown in Figure 2. In this section, the development of CPS will be overviewed within the framework of these three scales.

Conceptual process design and synthesis originate from the concept of unit operation. This concept was first introduced by A.D. Little in 1915. He pointed out that any chemical process may be represented as a series of ‘unit operations’ (King, 2000). Until the late 1960s, the unit operation concept was a cornerstone of process design, thanks to the works of Rudd and his students, and dealt with the synthesis problem using systematic approaches (Rudd and Watson, 1968). During the following twenty years, considerable research was performed in the area of process synthesis. At that time, most of the research was related to well-defined sub-problems. The developments made in CPS up to the mid-eighties can be briefly described as having been made at the **meso scale**.

The emergence of new “ macro factors”, such as the opening of global markets, the growing involvement of societies and governments in issues related to technology and the progress of the material and bio sciences, has re-focused interest in CPS on the macro and micro scales.

In the last decade of the 20th-century, the difficult economic situation, new regulations on sustainable development and environmental concerns (waste minimisation, environmental impact minimisation (EIM)) directed CPS towards concurrent design. In consequence, the objectives of CPS have been extended to a wide range of issues involving different disciplines; CPS has moved to the **macro scale.**

Traditional activities in the design and manufacture of bulk commodity chemicals are now organised with a significant focus on the design and manufacture of speciality, high-value-added chemical products. This change has required, among other things, the application of in-depth process knowledge within process design. It has resulted in the introduction of new,

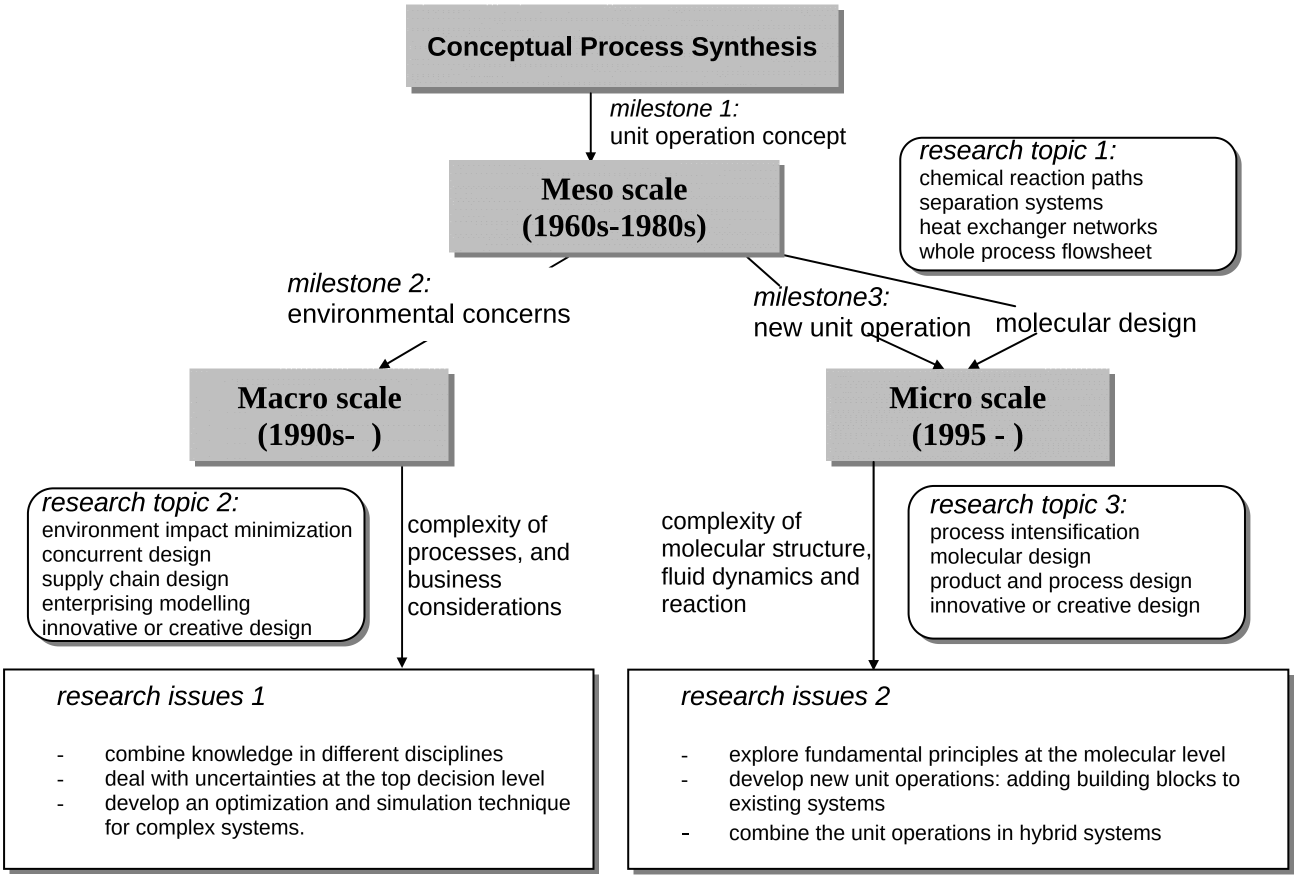


Fig. 2. The development of conceptual process synthesis

multi-functional units that ensure considerable process intensification as well as the extensive use of computer simulation at the particle and molecular level. The scope of CPS has expanded from issues of process design to ones concerning both product and process design. This re-focusing of interest has led CPS to move to the **micro scale.**

Figure 2 shows a combination of the micro, meso and macro scales of CPS associated with their current research issues. During the last decades, conceptual process synthesis at the meso scale has attained a high degree of scientific maturity. However, considerable further development is needed at the macro and micro scales. A more detailed review of work at the different scales can be found at the attached paper (**IX**) - chemical process synthesis: past and current trends.

2.3 The General Tasks of CPS

Regardless of the type of definition of CPS, design tasks are common to all kinds of design methods. A generalisation, which is still applicable, was first proposed by Motard and Westerberg (1978). They pointed out that there exist three important problems in process design and synthesis:

The representation problem – Is it possible to develop a representation that is rich enough to allow all the alternatives to be included and “intelligent” enough to automatically ignore ridiculous options?

The evaluation problem - Can the alternatives be evaluated effectively so they may be compared?

The strategy problem - Can a strategy be developed to quickly locate the best alternatives without totally enumerating all the options?

Considering recent developments and emerging research issues in process synthesis, new problems in relation to the above-mentioned become evident.

The representation problem - Can a representation be developed to enable the generation of new units and ways of processing?

The evaluation problem - Can different alternatives be effectively assessed using the life-cycle concept and multi-objective requirements?

The strategy problem - Can a strategy be developed to quickly locate better and innovative alternatives without enumerating totally all the options?

It is clear that the tasks of CPS are evolved in the way of satisfying multi-objective requirements and generating new solutions. Effective design methods and solutions are very dependent on the nature of the tasks to be addressed. The above-mentioned tasks are the basis to evaluate the methods of the conceptual design and synthesis.

2.4 Conceptual Design Methods

Traditionally, the design methods for CPS can be classified into two groups: optimization-based and knowledge-based methods. The main idea of the optimization-based approach is to formulate a synthesis of a flowsheet in the form of an optimization problem. It requires an explicit or implicit representation of a superstructure of process flowsheets from among which the optimal solution is selected. Knowledge-based methods concentrate on the representation and knowledge organisation of the design problem. In this section, the main emphasis is on knowledge-based methods.

2.4.1 Heuristic Approach

Heuristic methods are founded on the long-term experience of engineers and researchers. Rudd and his co-workers (Siirola and Rudd, 1971) made a first attempt to develop a systematic heuristic approach for the synthesis of multi-component separation sequences. In subsequent years, a lot of research was carried out based on this approach; e.g. (Seader and Westerberg, 1977). The hierarchical heuristic method is an extension of the purely heuristic approach and combines heuristics with an evolutionary strategy for process design. Douglas (1985) has proposed an hierarchical heuristic procedure for chemical process design where heuristic rules are applied at different design levels to generate the alternatives. During the design process, an increasing amount of information becomes available and the particular elements of the flowsheet start to evolve towards promising process alternatives. Shortcut calculations, based on economic criteria, are carried out at every stage of process design. The hierarchical heuristic method consists of the following steps:

Step 1. Batch vs. continuous.
Step 2. Input-output structure of the flowsheet.
Step3. Recycle structure of the flowsheet.
Step 4. Separation system synthesis.
Step 5. Heat recovery network.

The hierarchical heuristic method emphasizes the strategy of decomposition and screening. It allows for the quick location of flowsheet structures that are often ‘near’ optimal solutions. However, the major limitation of this method, due to its sequential nature, is the impossibility to manage the interactions between different design levels. For the same reason there are problems in the systematic handling of multi-objective issues within hierarchical design. The hierarchical heuristic method offers no guarantee of finding the best possible design. Smith et al. (1988) have proposed an onion model similar to the hierarchical heuristic model for decomposing chemical process design into several layers. The design process starts with the selection of the reactor and then moves outward by adding other layers – the separation and recycle system.

The heuristic approach has been used in many applications, such as the synthesis of separation systems (Seader et al., 1977; Nath et al., 1978), process flowsheets (Siirola and Rudd, 1971; Powers, 1972), waste minimisation (Douglas, 1992) and metallurgical process design (Linninger, 2002). Douglas (1988) illustrated the hierarchical heuristic method in detail using a case study of the synthesis for the hydrodealkylation of toluene (HDA) process.

2.4.2 Means-Ends Analysis

Siirola (1971, 1996) pointed out that the purpose of a chemical process is to apply various operations in such a sequence that the differences in properties between the raw materials and the products are systematically eliminated. As a result, the raw materials are transformed into the desired products. However, once a property difference is detected, it is possible that a prospective method may not completely eliminate the property difference. In such a case, another follow-up method for the same property difference may need to be specified. The undesirable side effects of the reduction of a property difference may also create, increase or decrease the differences of other properties. The hierarchy for the reduction of property differences is as follows: identity, amount, concentration, temperature, pressure and, finally, form.

The means-ends analysis paradigm starts with an initial state and successively applies transformation operators to produce intermediate states with fewer differences until the goal state is reached. However, not all properties can be considered for the overall flowsheet synthesis: only some of them may be considered while others are temporarily ignored. This property changing method is strongly limited as it ignores the influences and the impact on the other properties. Moreover, the search method takes an opportunistic approach, which cannot guarantee the generation of a feasible flowsheet.

The means-ends analysis approach was used as an early systematic process synthesis method for overall process flowsheet synthesis. It is based on the specification that both the initial state of the starting materials and the goal state of the desired products are known (Mahalec and Motard, 1977). Siirola (1996) illustrates the approach in the context of overall flowsheet synthesis as well as for the more detailed case of a separation system to resolve the concentration differences for non-ideal systems that include azeotropes.

2.4.3 Phenomena-Driven Design

Phenomena-driven design proposes that reasoning should not start at the level of building blocks but at a low level of aggregation, i.e. at the level of the phenomena that occur in those building blocks. Jaksland et al. (1995) studied separation process design and synthesis based on thermodynamic phenomena. They explored the relationships between the physicochemical properties, separation techniques and conditions of operation. The number of alternatives for each separation task is reduced by systematically analysing these relationships. Then, the possible flowsheets are produced with a list of alternatives for the separation tasks. From the viewpoint of the development of design methodology, Tanskanen and Pohjola (1995) proposed the following definition for ‘process design’: the ‘control of physicochemical phenomena for a purpose’. This design method takes the occurring phenomena as the ‘heart’ of the process, and the design tasks are decomposed at various levels by asking the following questions in sequence: what is desired, where can it be achieved (in which unit), when (under which conditions), and how can it be achieved (Gavrila and Iedema, 1996). The following hierarchical task levels correspond to the sequence presented above:
Task 1: role assignment
Task 2: phenomena grouping
Task 3: operating condition analysis (temperature and concentration analysis)

The decomposition process of this method proceeds along the hierarchical levels of precondition, action and influence of the process phenomena. It offers a systematic way of generating the desired phenomena and favourable conditions in order to implement the design objectives. Without the boundary of the unit operation, this method is aimed at exploring innovative units and processes to support creative design. However, the phenomena-driven method is based on opportunistic task identification and integration. The applicability of the methodology is demonstrated by its use in the design of an MTBE production process and reactive distillation system (Tanskanen et al., 1995).

2.4.4 Case-Based Reasoning (CBR)

Case-based reasoning imitates human reasoning and tries to solve new problems by reusing solutions that were applied to past similar problems. It deals with very specific data from previous situations and reuses results and experience to fit new problem situations. CBR is a cyclical procedure in nature. During the first step, retrieval, a new problem is matched against problems of previous cases by calculating the value of the similarity functions in order to find the most similar problem and its solution. If the proposed solution does not meet the necessary requirements of the new problem, CBR proceeds onto the next step, adaptation, and creates a new solution. The returned solution and new problem together form a new case that is incorporated in the case base during the learning stage.

The main disadvantage of CBR is the very strong influence of old designs and the lack of sufficient adaptation methods to support innovative design. CBR has been used for the design of distillation systems in process engineering (Surma and Braunschweig, 1996; Hurme and Heikkilä, 1999).

2.4.5 Optimization-Based Approach

Optimization-based methods use not only traditional deterministic algorithms, such as Mixed-Integer Non-Linear Programming (MINLP), but also stochastic ones such as Simulated Annealing (SA) and evolutionary algorithms such as Genetic Algorithms (GA). Two common features of these methods are the formal, mathematical representation of the problem and the subsequent use of optimization. A lot of studies have been carried out into this approach, and it has been widely applied in process design and synthesis. A recent review of the optimization based approach for process synthesis is given by Grossmann (1996, 2001).

The advantage of this approach is the provision of a systematic framework for handling a variety of process synthesis problems and the more rigorous analysis of features such as structure interactions and capital costs. An important drawback of optimization-based methods is the lack of the ability to automatically generate a flowsheet superstructure. Another disadvantage is the need for a huge computational effort and the fact that the optimality of the solution can only be guaranteed with respect to the alternatives that have been considered a priori (Grossmann, 1985). Therefore, this approach encounters great difficulties when dealing with the optimization of under-defined design problems and uncertainties that result from multi-objective requirements of the design problem.

2.4.6 Driving Force Method

Sauar et al. (1996) have proposed a new principle of process design based on the equipartition of the driving forces. They claimed that 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. However, Xu (1997) pointed out that the basic assumption that entropy production rates are proportional to the square of the driving forces is not valid for many important chemical processes. Although the fundamentals of this principle are the subject of discussion (Haug-Warberg, 2000), the potential importance of the method is hard to overestimate. Recently, Kjelstrup et al. (1999) described the design of a chemical reactor through the application of the driving force distribution.

2.5 Summary

Conceptual process synthesis has evolved from conventional process design at the meso-stage to the macro- and micro- stages. Industrial processes have to be designed and operated in a way to satisfy multi-objective requirements and generate new solutions. There is a trend to develop new concepts, techniques, and process with more attention being paid to this than to incremental improvements in the existing process. The challenges involved motivate research towards addressing, understanding and systematising the creative aspects of the process design. Thus, methodology to support the enhancement of creativity in process design is desired among both academia and industry.

3 CREATIVITY SUPPORTED METHOD FOR DESIGN

3.1 Creativity in Design

Creativity is the generation of ideas that are both novel and valuable. Generally, the concept of creativity covers a very broad range of artifacts like designs, theories, melodies, paintings, sculptures, and so on (Boden, 1999). Carr and Johansson (1995) gave the definition that creativity is the generation of ideas and alternatives; and the transformation of those ideas and alternatives into useful applications will lead to change and improvement. From the point of view of design, Rusbult (2003) pointed out that design is 'the process of using creativity and critical thinking to solve a problem'. Douglas (1988) proposed that process and plant design is the creative activity whereby designers generate ideas and then translate them into equipment and processes for producing new materials or for significantly upgrading the value of existing material.

From the point of view of the whole process life cycle, the opportunities for enhancing the creativity differ sharply. The earlier the stage, the greater the freedom for changes, i.e. there are more opportunities for enhancing the creativity of the design, and there is a lower cost for modification. If no attention is paid until the construction stage, even though many practical opportunities may still exist; the cost for retrofits will dramatically increase (Yang et al., 2000). This situation is illustrated in Figure 3. It shows that the key stage, in order to enhance the creativity and to reach the effective process solutions, lies in the conceptual design stages.

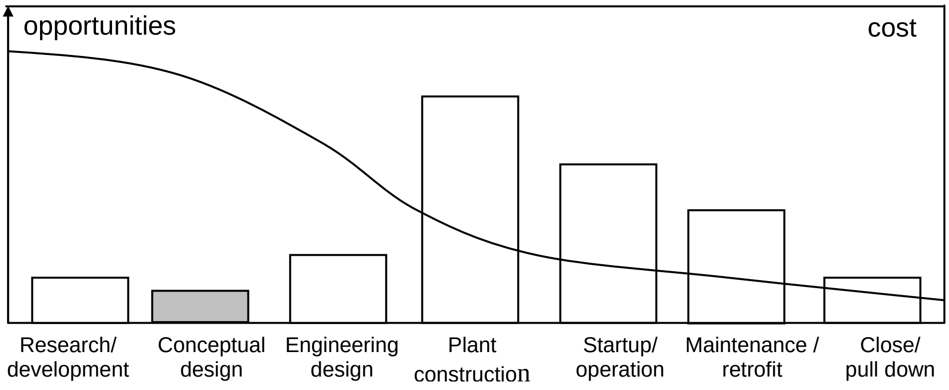


Fig. 3. Opportunities for improving creativity along the process life cycle

3.2 Modes of Creativity for Design

Many methods and techniques to stimulate creativity exist, along with the development of various procedures and processes. Here the methods of enhancing creativity for design are classified into three modes: ‘imitational’, ‘combinational’ and ‘systematic’ mode. Imitational creativity is found in the engineering approach to enhancing creativity along the traditional ways of pursuing either psychological or imitational paths. The methods belonging to this class are brainstorming and synectics. Combinational creativity focuses on unusual combination or association between familiar ideas. Examples are attribute listing, morphological analysis, and case-based reasoning. Systematic creativity, the last group, is a practical approach to enhancing engineering creativity. The term ‘systematic creativity’, according to Mann and Dewulf (2002), means that the aim of this methods is to make the problem solving process progress from the random to the systematic, while keeping and exploring all possibilities of good solutions. Systematic approaches to support design problem solving and to improve the design quality have been developed, such as theory of inventive problem solving (TRIZ) and axiomatic design (AD). Those methods are presented in more detail in the following sections.

3.2.1 Imitational Mode

The purpose of imitation-based methods for engineering design is to elicit the ideas of the individual. The approach explores novel and multiple possibilities and approaches instead of pursuing a single approach. There are several popular methods used for engineering design. Brainstorming is one of the earliest attempts to develop a structured approach to the enhancement of creativity and started with the works by Osborn (1963). This technique, designed specially for use in groups, encourages participants to express ideas, no matter how strange they may seem and forbids criticism during the brainstorming session. It could generate a large number of ideas, most of which will be subsequently discarded, but with perhaps a few novel ides being identified as worth following-up (Nickerson, 1999). Another method is synectics introduced by Gordon in 1961. It is similar to brainstorming, however, it uses analogical thinking and the group of participants tries to work collectively towards a particular solution, rather than generating a large number of ideas (Cross, 2000). Another approach is based on so-called lateral thinking. It was proposed by de Bono in 1967 (Bono, 2003) and is concerned with the perception part of reasoning. It is about moving sideways when working on a problem to try different perspectives, different concepts and different points of entry.

3.2.2 Combinational Mode

The essence of the combinatorial mode is to search for possible solutions by combining the various aspects of old solutions. Association and analogy are examples of combinational creativity (Boden, 1999). The association methods, such as attribute listing and morphological analysis, concentrate on splitting the original problem into smaller sub-problems and then examining various aspects of the solutions to the sub-problems. Then the possibility of combining solutions to generate new solutions is considered. Morphological analysis is an extension of attribute listing. It is an automatic method of combining parameters into a new combination for later review by the problem solver. A selection of parameters or attributes is chosen and combinations are explored (Larson and Minn, 1977). The Arrowsmith method is one of the association methods. The aim is to search for hidden patterns and predictive information based on an available literature database. The main idea of this method is as follows: fact A is related with fact B, and fact B is related with fact C. Simultaneously it is assumed that there is a relation between A and C and this relation is explored (Kostoff, 1999).

The main issue with the analogy-based methods is to find the similarity among the problems and then adapt old solutions to the new problems. An example is cased-based reasoning (CBR). CBR imitates a human reasoning and tries to solve new problems by reusing the solutions that were applied to past similar problems. It deals with very specific data from previous situations, and reuses results and experience to fit a new problem situation.

3.2.3 Systematic Mode

The main focus of these methods is on the reduction of ineffective solutions by using a purposeful and systematic procedure. This group of methods is the most practical and applicable approach to support engineering design (Leobmann, 2002). They can overcome inertia caused by routine engineering behaviour and insufficient knowledge of a given topic. The systematic approaches include methods such as AD and TRIZ.

An axiomatic approach to design is used to define both a design methodology and a set of rational criteria for decision-making (Suh, 1990). The method is based on two axioms. The first one is the independence axiom. It states that good design maintains the independence of the functional requirements. The second one is the information axiom. It claims that in a good design the information content is minimised. It establishes the information content as a criterion for the evaluation of the design alternatives. Leonard and Suh (1994) presented the concept of axiomatic design as a framework for concurrent engineering. This methodology has been discussed for the design of manufacturing systems, material-processing techniques, and product design (Suh, 2001).

TRIZ is a method of the identification of a system's conflicts and contradictions aimed at the search for the solutions of inventive problems (Altshuller, 1998). The main idea of TRIZ consists of the modification of the technical system by overcoming its internal contradictions. Compared with other methods, TRIZ (and TRIZ-based methodology) is the only innovative knowledge-based and evolutionary-directed technique (Zusman, 2000).

3.3 TRIZ method

Mann (2002) stated that TRIZ is a philosophy, a process and a series of tools. Figure 4 illustrates a hierarchical perspective of TRIZ. It shows that the TRIZ method is based on the round foundation of design knowledge and a large amount of research study. TRIZ philosophy states that 'problem solving is the process of identifying and removing the conflicts in order to evolve the system towards the increase of ideality'. There are two essential concepts: contradiction and ideality. According to the dialectics, contradiction within a thing is the fundamental cause of its development (Savransky, 2000). The problem is originated from the contradictions between its characteristics. Ideality is a general trend of behaviour of all systems. It consists in increasing the benefits of the system while reducing both the disadvantages and cost (what is TRIZ, 2000).

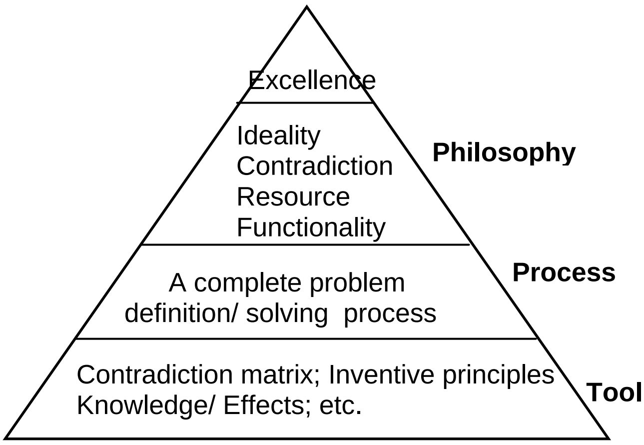


Fig. 4. Hierarchical view of TRIZ (Mann 2002)

Savransky (2000) gives a definition of TRIZ from the point of view of engineering: TRIZ is a human oriented knowledge-based systematic methodology of inventive problem solving. ‘Knowledge’ here is the generic problem-solving heuristics which is extracted from a vast number of patents worldwide in different engineering fields. ‘Human oriented’ means that those heuristics are formulated and operated by a human being, not a machine. ‘Systematic’ emphasizes that the procedure for problem solving and the heuristics is structured in order to provide effective application of known solutions to new problems. And ‘inventive problem solving’ implies that the problem solving can signal the most promising strategies without missing any good solutions.

TRIZ methods have been proved to be a useful method for exploring ideas and solutions systematically. A systematic programme, which compares the different creativity tools, methods and concepts in terms of their relevance to primarily scientific, engineering, and business applications, has concluded that TRIZ currently offers the most useful foundation for a systematic creativity model (Mann, 2000). The applicability of TRIZ has been tested by the enterprises. For example, MGI Company has concluded that TRIZ methodology is the most suitable method for the generation of design alternatives and selection of design techniques (Cavallucci et al., 2000). The advantages of TRIZ methods have been discussed in many articles (Cavallucci et al, 2002; Zusman, 2000; Mann, 2000). In summary: TRIZ is a method which

- guarantees a degree of reliability so that the design phases are planned with accuracy.
- benefits from the knowledge capacity to generate ideas systematically when these are lacking.
- includes the ability to overcome the psychological inertia of experts in the field.
- guarantees clarity and understanding of the solutions generated.

Much research work has been done on the application of TRIZ tools to design, particularly product design. (Low, et al., 2000; Goldenberg et al, 2002). However there is no meaningful, published application for the process industry, although Poppe and Gras (2002) have pointed out that TRIZ has aroused increasing interest in the process industry. They emphasized that extra care has to be given to the analysis and modelling stages when applying TRIZ to process industry. There are two main ways for adapting TRIZ tools to process applications: one is to study the application of the generalized tools of TRIZ, for example the application of inventive principles (Winkless et al., 2001,) and problem solving tools (Freckleton, 1999). Another is to adapt the concepts and problem solving strategies of TRIZ for a specific problem domain, like the application and integration of TRIZ strategies for problem solving (Baessler et al., 2002; Leon-Rovira et al., 2000).

3.4 Summary

Enhancing the creativity of design is becoming an essential issue in process design. Various methods exist to enhance creativity in engineering design. Considering the evolutionary nature and knowledge intensive features of process design, enhancement of creativity is towards the way of ‘systematic creativity’. TRIZ, the systematic approach, is promising for adaptation to the development of a process design method. The concepts and problem solving strategies of TRIZ are the foundations for developing creativity-supported methods for chemical process design.

In this work, three aspects are highlighted to enhance the creativity for chemical process synthesis from the viewpoint of the development of design methodology. They are based on the characteristics of the TRIZ method and the nature of conceptual process synthesis.

- The new concept for presenting the design problem stimulates the ability to understand and analyse design problems.

The new concept is able to represent the design targets and tasks considering the requirements of multi-objective criteria. It helps designers understand all aspects of the design problem.

- The organized design knowledge assists decision-making for both design experts and novices.

The knowledge base can collect all available design heuristics and experience, which overcomes the limitation to decision making caused by insufficient design knowledge.

- The new design paradigm guides the design activities in the context of the whole process synthesis both for early and detailed design.

It bridges the gap between the design activities at the early design stage and the detailed stage; an issue which is not addressed with existing design methods. Consequently, the efficient and compact solution space built at the early design stage can improve the efficiency of solution optimization in the detailed stage.

4 CONFLICT-BASED METHOD FOR CONCEPTUAL PROCESS SYNTHESIS

4.1 Overview of the Methodology Development

This section presents a systematic study of the development of a methodology in order to investigate a creative supported approach for process synthesis. The aim is to support decision making in design and synthesis, especially to handle the multi-objective requirements and combinatorial nature of process synthesis. The development of the methodology deals with two main questions: how to define and identify the conflicts encountered in the design process; and what are the strategies and procedures to resolve the contradictions and to improve the process performance with regards to multiple design objectives.

The work is based on the Theory of Solving Inventive Problems (TRIZ). Figure 5 shows an outline of the development of the methodology for conceptual process synthesis based on TRIZ concepts, tools and strategies. There are two groups of tasks corresponding to the above-mentioned questions: the first is to define the design tasks in the light of the concept of conflict; the second is to investigate the conflict-based paradigm for modelling the design activities of problem solving.

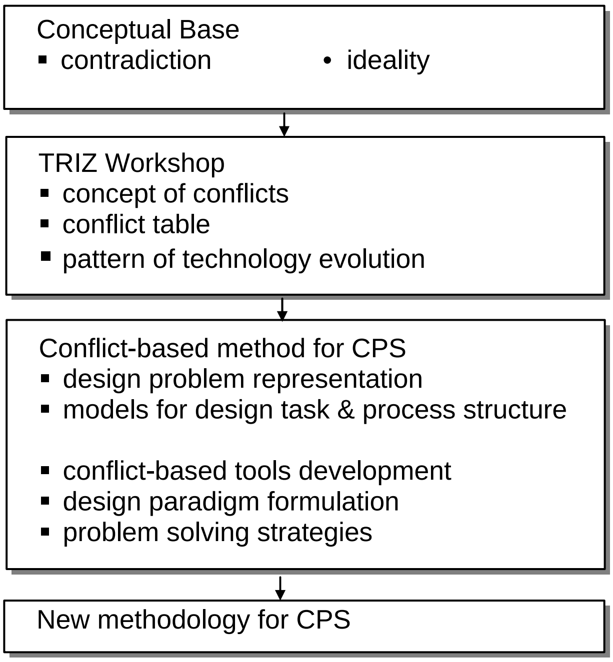


Fig. 5. TRIZ environment for methodology development of CPS

4.2 Design Tasks in the Context of Conflicts

To develop the methodology for process synthesis, it is essential to understand the design tasks from the viewpoint of the concept of conflict. This section deals with the following issues: the concept of conflicts in chemical process synthesis; a definition of process synthesis based on the concept of conflict; the conflict model for problem representation and knowledge organization; and, the structural model of process to support conflict-based analysis.

4.2.1 The Concept of Conflicts

It is stated that TRIZ is an approach to identify a system’s conflicts and contradictions to solve inventive problems. The main idea of TRIZ consists in the modification of the technical system by overcoming its internal contradictions. The contradictions occur when improving one parameter or characteristic of a system negatively affects other parameters or characteristics of the system.

For chemical process synthesis, the conflicts occur not only among the multi-objectives but also among the characteristics of the process. It is obvious that the multiple objectives of process design are always conflicting since an improvement in one objective cannot be obtained without deterioration in others. For example, an exclusively profit-driven criterion may lead to a solution with negative environmental impact. The major challenge of multi-objective design and synthesis lies in resolving the objective conflicts to achieve optimised solutions (Miettinen, 1999). Therefore the design targets could be represented by conflicts among the multiple objectives. Moreover, the chemical process design is aimed at realizing or improving the required performance of the process flowsheet through identifying the types of units, their interconnections and the optimal parameters. Improving the performance of process flowsheets must be based on changes in the characteristics of the chemical process, such as chemical and physical properties, the topology structures, etc. The changes in the process characteristics concerned always result in changes in other process characteristics because of design constraints and specifications. The design activities need to handle the conflicts among the improved characteristics and the correspondingly changed ones. All these conflicts are the precondition for developing the conflict-based method for CPS. Then there occurs the question:

- *How to define conceptual process synthesis based on the concept of conflict?*

To answer this question, it is necessary to understand the definition of process synthesis.

4.2.2 Definition of Process Synthesis

TRIZ states the definition of problem solving as below:

Problem solving is the process of identifying and removing the conflicts in order to evolve the system towards the increase of ideality.

According to TRIZ, the most effective inventive solution to a problem is often the ones that overcome the contradictions. The conflict is the driving force of problem solving which represents the design problem and controls the problem solving. The ideality is the criterion of design quality or evaluation criteria.

Process synthesis is a complex problem solving process based on qualitative, semi-qualitative and quantitative information as well as multiple objective design criteria. In view of the conflict concept, three types of problems are classified; the characteristics of their corresponding decision-making types and solutions are as listed in Table 1. For well-defined problems, when there are no conflicts, the decision-making is done in a predetermined way. This results in specific and routine solutions. When there are conflicts for certain problems, the decision-making can be done based on well-founded principles of process engineering and the obtained solution will also be specific and routine. However, most synthesis problems are open-ended and under-defined, often with the existence of conflicts. The decision-making involves trade-offs for problem solving. Those are the most complex and difficult tasks. Therefore they are the main subject of research and the main sources of the various design alternatives and creative solutions. The research work in this thesis deals with this group of problems. The following is a definition for process synthesis in the context of conflicts:

Process synthesis is the decision-making process of identifying and handling the conflicts in design in order to satisfy the multi-objective requirements.

Table 1. The classification of design problems

Design problems	**Decision Making**	**Solutions**
Well defined, no conflict	Determinate	Specific, routine
Well defined, conflict	Determinate	Specific, routine
Under-defined, conflict	Trade-off	Several alternatives, creative

There are two concepts in the definition, which should be explained in more detail: conflicts, and their handling. The identified conflicts represent the design problem. Conflict handling means the design activity of operating or removing the conflicts in the design in order to satisfy the design requirements and criteria.

Based on the definition, one critical question emerges:

- *How to represent the process synthesis problems in the conflicts*

To answer it, the conflict model for problem representation is proposed.

4.2.3 Conflict Model of Problem Representation

Dym (1995) claims that representation is a key issue in process design. Representation is not an end in itself but a means to an end; it is a way of setting forth a situation or formulating a problem so that an acceptable resolution to a design problem can efficiently be found. Representation can clearly state the design targets and tasks and also support design knowledge management. It assists problem solving and evaluation in following design stages as well.

The conflict model is proposed for the representation of the design targets and problems. It allows the decomposition of design targets and the organization of design knowledge. As mentioned above, there are two groups of conflicts encountered during the design process: one is the conflict among the multiple objectives; the other is the conflict among the process characteristics, such as process parameters (operating parameters and process structure elements). It is clear that the two groups of conflicts are related to each other: The former is the effect or function of the latter. However their interactions are difficult to describe precisely because of the complexity and combinatorial nature of chemical processes. In order to bridge the gap and simplify the functionality between the two abstract levels of the design targets and the process parameters, a medium level of conflicts is proposed - the conflicts among the process properties. The process properties are the

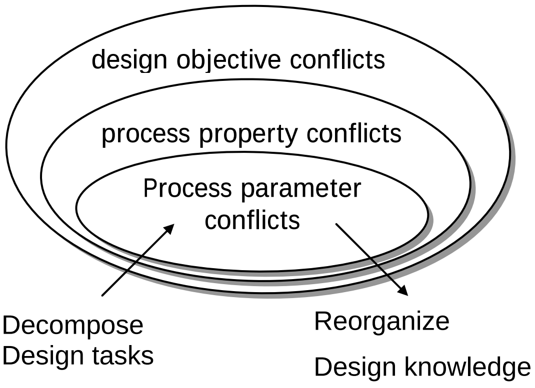


Fig. 6. Conflict model

performance of the process blocks or process phenomena, such as the reaction conversion, reaction selectivity, separation efficiency, etc. The process properties are the combination or function of the operating parameters. So the conflicts among design objectives are the effect of conflicts among the process properties, which are the function of the process parameters. The conflict model for process design is made up of three functional levels.

Figure 6 shows the proposed conflict model. From the outer level to the inner level, it illustrates the decomposition of design targets or tasks: design targets are presented through the conflicts among the concerned design objectives. To handle these conflicts, the sub design tasks which are essential for the design target are identified. And the conflicts are transferred to the ones among the process properties simultaneously. The process properties relate to the process blocks and phenomena. The conflicts of the process properties are originated by the trade-offs among the values of the process parameters. So the conflicts are moved to the level of the process parameters. They are directly influenced or operated by design knowledge and heuristics. As a result, the transfer of the conflicts from outer to the inner level is carried out with the decomposition of the design tasks into the subtasks. The conflicts are formulated to represent the design tasks at different levels of process design.

From the inner level to the outer level, the model shows the way the design knowledge is organized and analysed. First, applying the design knowledge and heuristics will directly affect the process parameters. It identifies the conflicts among the process parameters; then the changes of the parameters will result in conflicts among the process properties. Consequently, conflicts of design objectives occur because of the changes of the process properties. Therefore, the design knowledge and heuristics are analysed and the effect of their application to the three levels of conflicts is studied. The affected design objectives and the implicit information behind the design knowledge are extracted. It is an approach to the structuring of conflicts-oriented analysis for the organisation of the design knowledge. It is also the main idea behind building the conflict-based tools which will be discussed in the next section.

The proposed conflict model is an abstract approach to provide a way of task decomposition and knowledge organization. Next a structural model of process flowsheet to support conflict-based analysis is proposed and the question below answered:

- *Where to apply the conflict model?*

4.2.4 A Structural Model of Process Representation

Process synthesis relies heavily upon a robust superstructure. Conflict-based analysis for process synthesis is rooted in the process structure. The initial process structure could be represented by the existing blocks and units. For the conflict-based analysis of the reactor and separator network, in this work, the system is represented by the proposed phenomena structure.

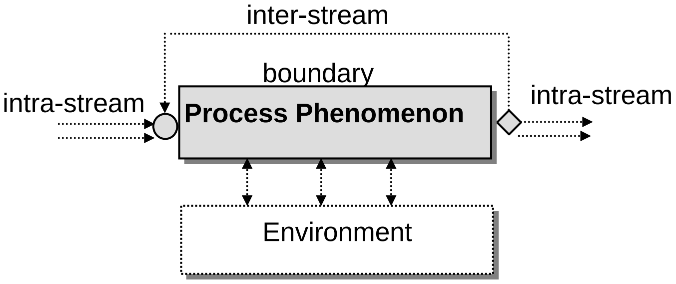


Fig. 7. The generic phenomena structure of RS

Complex plant connectivity is an important structural issue for the synthesis of a reactor and separator (RS) network. Most design methods combine and configure existing building blocks when searching for solutions. The drawback of this approach is that the solution is limited by the types of existing blocks. Really new and creative solutions will mostly not be found in this way. Therefore, it was recently suggested that reasoning should not start at the level of building blocks but at a low level of aggregation, the phenomena occurring within the building blocks (Tanskanen et al., 1995). In this work, a generic phenomena structure for a reactor and separator system is proposed as shown in Figure 7, without considering any type of units and their number. It includes the boundary, input mixer and output splitter. The boundary classifies the different phenomena, such as feeding, reacting, separating, recycling, etc. It is characterized by process properties, like reaction conversion, reaction selectivity, and separation efficiency. The input mixer collects the streams and output splitter distributes the streams of the related process phenomena. There are two types of streams: intra-streams and inter-streams. Intra-streams establish the connections between the mixer and splitter among the different phenomena; inter-streams establish the connection between the mixer and splitter of similar phenomena.

Conflict analysis for a RS system is based on the generic phenomena structure. Two places in this generic structure are identified which ‘store’ the conflicts or design problems:

- At the input mixer and output splitter. This is because the number of streams or interconnections of streams result in an imbalance in the process structure. In this case, the design problems then relate to the interconnection and the integration of the various phenomena. Here handling the conflicts of the design problem will determine the structural issue of the process synthesis.
- At the boundary between process phenomena and its environment. The reason is that the boundary properties are over the limits of the design specification, process constraints or produce mutually exclusive effects on the environment. The design problems then relate to the determination of the properties of the intra- and inter- streams concerned. Dealing with these conflict will determine the process parameters.

Applying conflict-based analysis to the process structure (initial structure or phenomena structure), the design tasks are described through the different levels of conflicts. By handling these conflicts, promising process alternatives or an efficient process superstructure evolve. Now a question related with the design activities arises.

- *How to handle the conflicts?*

4.3 Conflict-based Design Paradigm

This section presents the implementation of design activities via the conflict-based method. Firstly, general design activities are explained in the view of the concept of conflict. It shows that the conflict-based method can handle the design tasks of conceptual process synthesis. Then a design paradigm is formulated based on the classification of the conflicts with a hierarchical organization. Strategies for problem solving are proposed to support decision-making. The design tools, the conflict table, are constructed.

As a result, the conflict-based method is implemented through the modelling of the design activities. The method guides the decision-making towards the way of minimizing the number of the conflicts during the design process. It supports the generation of possible design alternatives or flowsheet superstructure in a systematic way.

4.3.1 Generic Process Design Paradigm

Siirola (1996) proposed the general design paradigm for conceptual process design shown in Figure 9. It is a four-step design procedure: formulation, synthesis, analysis and evaluation. At the formulation step, the process specification and objective criteria are defined. Then this is followed by an iteration of three steps: generation of an alternative (synthesis), determination of the behaviour of the alternative (analysis), and comparison of the performance of the proposed alternative against the goals and specifications presented at the formulation step (evaluation). This procedure naturally caters for the cyclic nature of a systematic creativity process. According to Mann (2002), a systematic creativity process is achieved through four basic steps by TRIZ methodology: ‘define’, ‘select’, ‘solve’ and ‘evaluate’. As illustrated in Figure 8: define what the problem is (conflicts); select the tools and models to support problem solving (contradiction matrix, etc.); generate problem solutions, and evaluate the solutions as the final step (ideality). Therefore the process design activities can be described as a systematic creativity process. It emphasizes the adaptation of the concepts and tools of TRIZ to carry out process design activities.

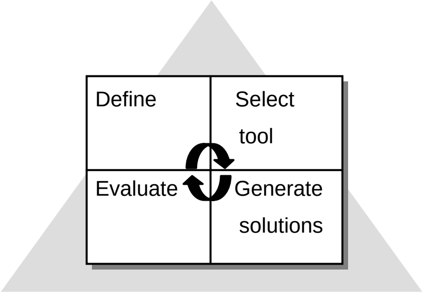


Fig. 8. Four basic steps of the systematic creativity process

For the early design stage, there is a high possibility that conflicts will occur among the objectives and process characteristics. This is due to the fact that at the early design stage there are complex design uncertainties as well as a huge decision space. The synthesis task is to remove or decrease the occurrence of conflicts through a proper decision-making process. The conflict-based model and conflict-based tools are applied to support the decision-making. As a result, possible process alternatives are generated to build the solution space. Process analysis is for analysing the various structural options and trade off the process parameters. The aim is to screen and modify the solution space, and to generate useful information. The modified solution space are applied for the next stage - the detailed design stage, where optimization and simulation are carried out to trade off the process parameters and search for optimal solutions. Then the process state is determined. The process evaluation is the final step in the examination of the process performance. The aim is to determine the optimal solutions. The design activities are iterated by two-optimization loops, where structure optimization takes place in the outer loop and state optimization in the inner loop. Therefore, the design activities, from the view point of the conflict concepts, are implemented along the framework of the generic design paradigm shown at Figure 9. This provides the foundation for developing the conflict-based design paradigm.

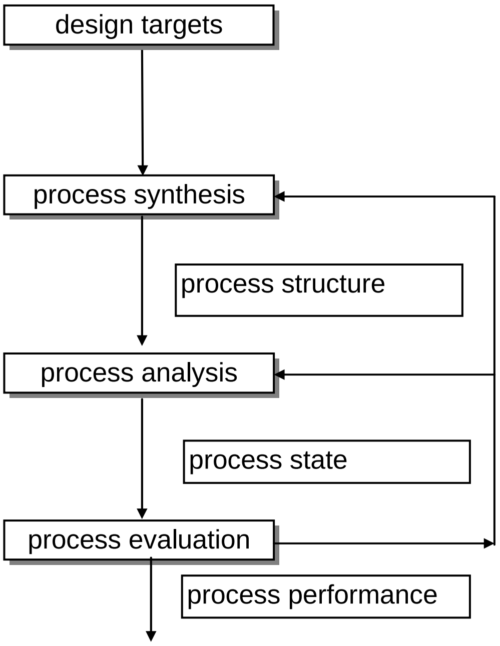


Fig. 9. The general design paradigm

4.3.2 Classification of Conflicts and the Hierarchy

The classification of conflicts and their hierarchy is the precondition for developing the conflict-based design paradigm. TRIZ (Savransky, 2000) classifies two groups of conflicts: system conflicts (SC) and physical conflicts (PC). System conflict is a situation where changes in one part of a technological system cause the deterioration of another part of the system. A physical conflict is a situation where one object has mutually exclusive physical states. This can be stated as ‘to perform action A1, the element must have property P, but to perform action A2, it must have the opposite property –P.

According to the conflict model, three levels of conflicts are identified: conflicts among the multi-objectives, conflicts among the process properties, and conflicts among the process parameters. The upper level mostly corresponds to the system conflicts since the improvement of one objective usually deteriorates others. The lower level is usually related to the physical conflicts due to the common functions, process specification and constraints. For example, by increasing the temperature of the reactor, the reaction conversion is increased. However, the reaction conversion is decreased with the change of feed concentration. The conflict between these two process parameters is a physical conflict. The conflicts among the process properties are usually related to both kinds of conflicts. It is because, in the one hand, the properties could contribute to the common objective function, and on the other hand, they require the opposite tendency of changes for process parameters. For example, when there exists side reactions of producing by-product, increasing the temperature will improve the reaction conversion, while decrease the reaction selectivity. The conflict of reaction conversion and selectivity belongs to the group of physical conflicts. Another example, in the view of improvement of environmental impact, is the beneficial effect of increasing the recycle ratio of the by-product. However this results in a decrease in the reaction conversion because of the reversible reaction. The conflict of these two properties is a system conflict.

According to TRIZ (Savransky, 2000), system conflicts cannot be eliminated directly. Handling of system conflicts is aimed at identification of the essential elements which control the competing attributes. Through modifying these elements the system conflicts will be transferred to physical conflicts. As shown in Figure 10, TRIZ gives the paradigm of problem solving for handling the system and physical conflicts. Figure 11 shows the conflicts transfer in a reactor/separator system design and synthesis. The hierarchy for identifying and handling conflicts is determined by the levels of the conflict model: first, the conflicts among the design objectives; then the conflicts among process properties; and finally the conflicts of process operating parameters such as stream properties and thermodynamic properties.

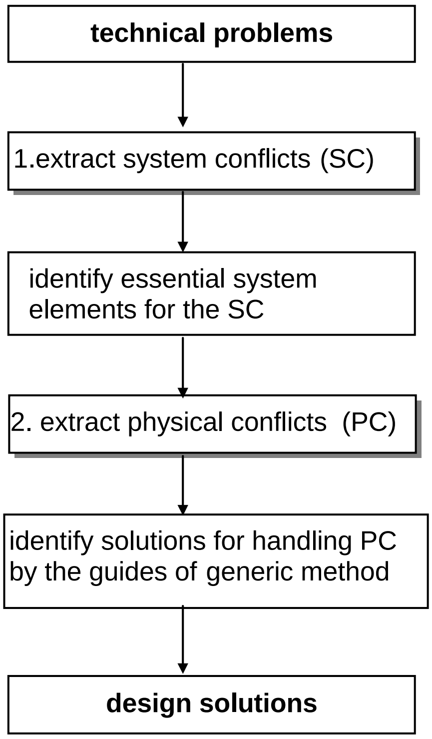


Fig. 10. The paradigm of TRIZ for general technical problems

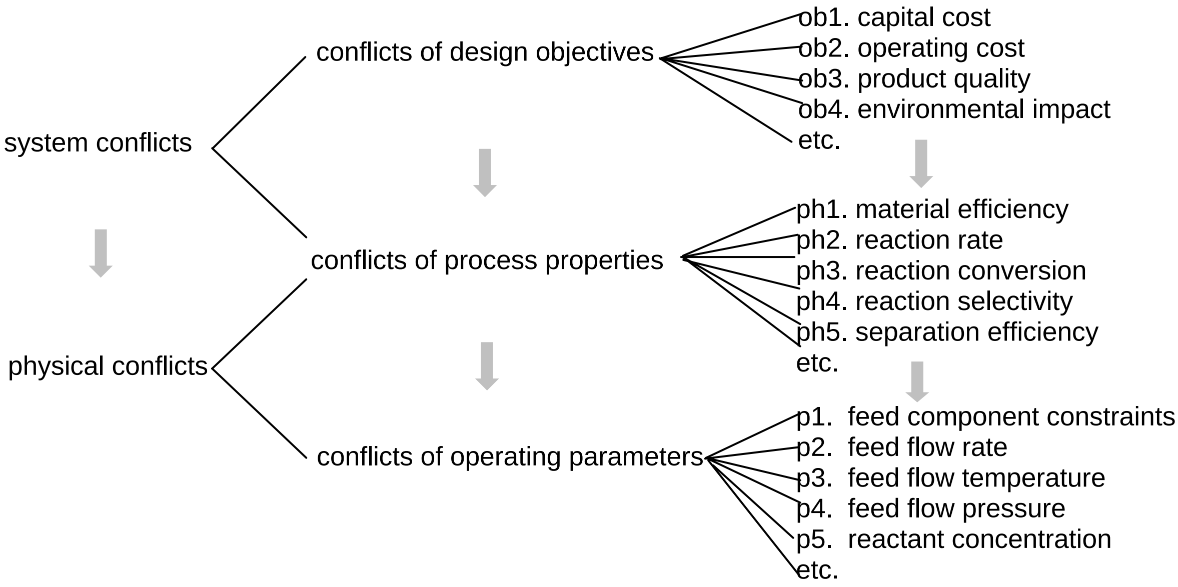


Fig. 11. Conflicts transfer in a RS system

4.3.3 Development of Design Paradigm

For chemical process synthesis, the design paradigm is formulated by combining the TRIZ strategy (Fig. 10) and the general process design paradigm (Fig. 9). The procedure consists of three steps for the whole conceptual process design as illustrated in Figure 12 marked by grey boxes: conflict-based analysis, process analysis, process simulation and optimization.

First, the conflicts among the objectives present the design tasks; For example, when improving the process profitability, it brings out negative impact for the environment. Therefore there is the conflict between process profitability and environmental impact. To handle the conflicts of the objectives, the sub design task or possible major structural issues are identified; By-product treatment is one of the important issues for handling the above conflict. Concerning with this sub task, the conflicts among the process properties are identified, such as the recycle ratio and raw material utilizing efficiency. Next these conflicts are transferred to the conflicts among the process parameters, which relates with stream properties and thermodynamic parameters; In order to handle the conflicts between recycle ratio and raw material utilizing efficiency, it is essential to trade off those parameters like the stream parameters of the recycle flow, the parameters of the raw material properties, and the operating parameters of reaction. The conflicts among these parameters are handled by selecting the suitable heuristics based on the supported design tools. As a result, promising process alternatives are generated which are subject to process analysis in the second step. The methods of thermodynamic analysis or qualitative reasoning are proposed for process analysis to modify the solution space. The solution space is the basis for searching of the optimal solutions in the final step through simulation or optimization. This procedure is iterated by solving the conflicts of process characteristics in the inner loop and by identifying the sub tasks of design in the outer loop. The optimal solutions are achieved until no further improvements to the generated flowsheet can be made.

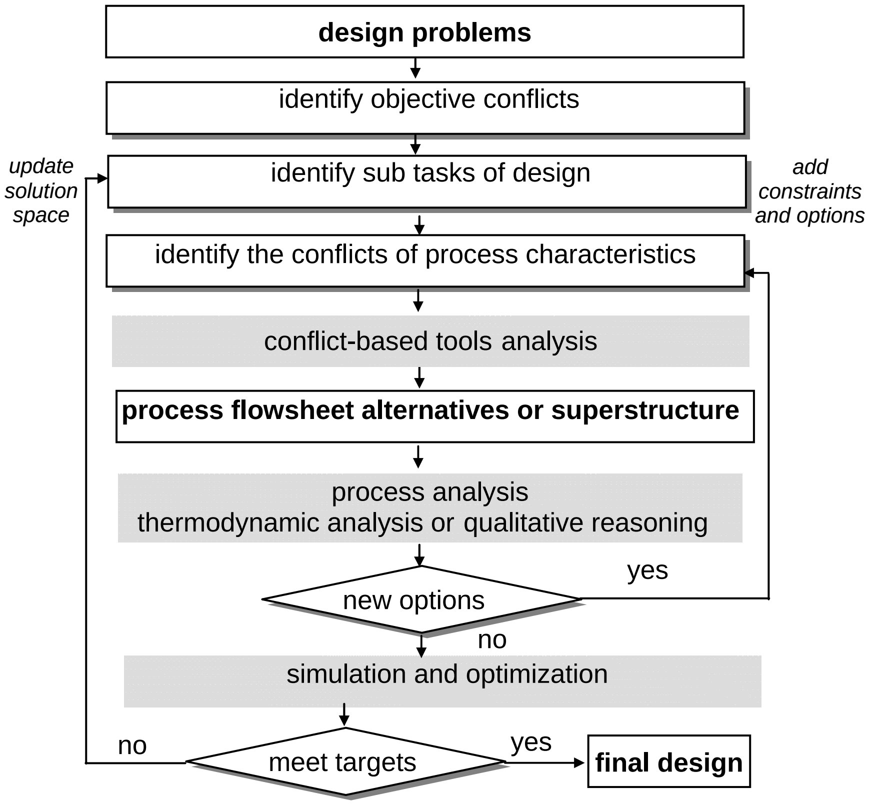


Fig. 12. The paradigm of conflict-based method for chemical process synthesis

The conflict-based method is used for generating and screening promising alternatives at the early stage of conceptual design. It can overcome the limitation of inappropriate decisions for multi-objective design caused by the narrow design space or insufficient design knowledge. The multi-objective requirements are considered at the early design stage. Identifying and removing the conflicts in a hierarchy way realize decision-making based on the minimization of the number of the conflicts during the design process. The solution space from the conflict-based method builds the foundation for the process analysis via thermodynamic analysis tools or qualitative reasoning. Process analysis could provide the useful information to bridge the gap between the qualitative knowledge and quantitative techniques. It assists the simulation and optimization stages in the search for the optimal solutions.

4.3.4 Extraction of Problem Solving Strategies

When applying the conflict-based method to chemical process synthesis, two strategies are proposed as the design criteria of conflict-based methodology. They are adapted from the axiomatic design introduced by Suh (1990). The basic postulate of the axiomatic approach to design is that there are fundamental axioms that govern the design process. Two axioms are identified by examining the common elements that are always present in good designs. They are also identified by examine actions taken during the design stage that resulted in dramatic improvements (Suh, 2001). The axioms are presented as design principles. The first is the independence axiom. It states that good design maintains the independence of the functional requirements. The second is the information axiom. It claims that in a good design the information content is minimised. To make the design work, the supplied information content is finite. By defining the information content in terms of probability, the second axiom states that the design that has the highest probability of success is the best design. It establishes the information content as a criterion for evaluation of the design alternatives.

In view of the conflict-based concept, the below two problem solving strategies are described:
Strategy 1: identify the conflicts among the less correlated process characteristics.
Strategy 2: select or apply design heuristics to result in the minimum number of conflicts.
Strategy 1 states that the identified conflicts, which characterize the design targets and problem representation, are less related or relatively independent. The aim is to avoid coupled design since coupled design will result in less promising design and requires unnecessary iteration of design parameters. For example, when dealing with the design task of the heat exchanger network, there often occur the conflict between reboiler number and the temperature profile, and also conflict between reboiler number and pressure profile. Since temperature and pressure are correlated parameters, one of these two conflicts is picked up as the design target. Therefore, this strategy guides the selection of conflicts towards to the direction of the independent functional requirements. Then Strategy 2, minimizing the number of conflicts, is used to decrease the iteration of problem solving. The aim is to minimize the content of information. It is obvious that new conflicts are brought out

sequentially when handling the upper level of conflicts. The strategy guides the decision making in current design level in a way of resulting in fewer conflicts for the following design level. Take the following case for instance: when economic criteria and process controllability are considered as the design targets for the waste minimization issue, there are suggested three heuristics concerning with the change of raw material condition. Heuristic of material substitution is screened out since it will results in more unexpected control problem, comparing with other heuristics, such as material purification and material updating quality.

4.3.5 Development of Conflict-based Tools for CPS

The development of TRIZ was first initiated by Genrich Altshuller (Altshuller, 1998) with his perception that invention is nothing more than the removal of a technical contradiction with the help of certain principles. The development of TRIZ tools is based on revealing similarities and common patterns between design problems and solutions published in patents. After studying 200,000 patents, Altshuller concluded that there are about 1,500 technical contradictions that can be resolved relatively easily by applying fundamental principles. With these he developed 40 universal principles for any technical system. He also identified 39 universal characteristics of technical systems that generate contradictions. With the 40 principles and 39 characteristics, he developed a contradiction matrix that could be used to solve contradictions generated by any technical system.

Similarly, based on the available literature in a specific domain, the process characteristics and design heuristics for building the design tool – the conflict table – are extracted. The tables have been developed for the design domains of distillation systems and reactor/separator systems, and waste minimization (APPENDIX **I-III**).

The precise format of the conflict table can differ in order to efficiently support problem solving and problem debottlenecking. The procedure for constructing the conflict table involves 5 steps as shown in Figure 13.

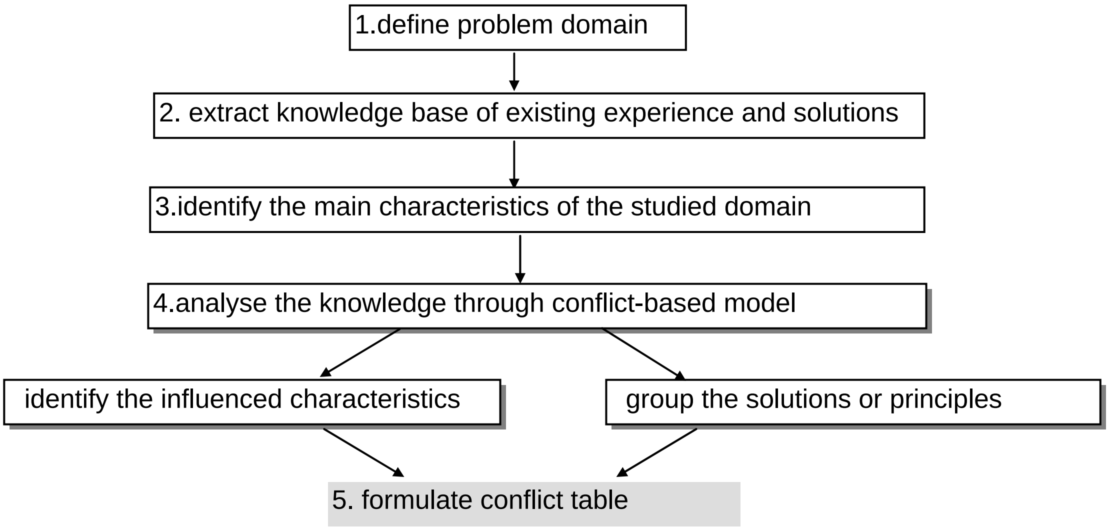


Fig. 13. The procedure of building the conflict table.

Here explains the above procedure together with the example of how to build the conflict table for the RS system.

Step 1: define the problem domain where a large amount of design heuristics, experiences and cases studies exist.

Multi-objective process synthesis of reactor and separator system is one of the important issues of the chemical process design. Much research work has been done to address this problem.

Step 2: extract the design heuristics from available literature which has been proven to be critical for the conceptual process design.

86 design heuristics are extracted from the available literatures which are mainly based on the work of Douglas (1988) and Smith (1985).

Step 3: identify the characteristics of the studied system based on the conflict model.

8 design objectives are selected which are often concerned for RS system, such as capital cost, operation cost, product quality, environmental impact, etc. There are identified 11 parameters of process properties which has the directly influence on the objectives, like raw efficiency, reaction conversion and selectivity. By analyzing the heuristics, 20 operating parameters are extracted. Figure 14 illustrates the parameters of building RS conflict table.

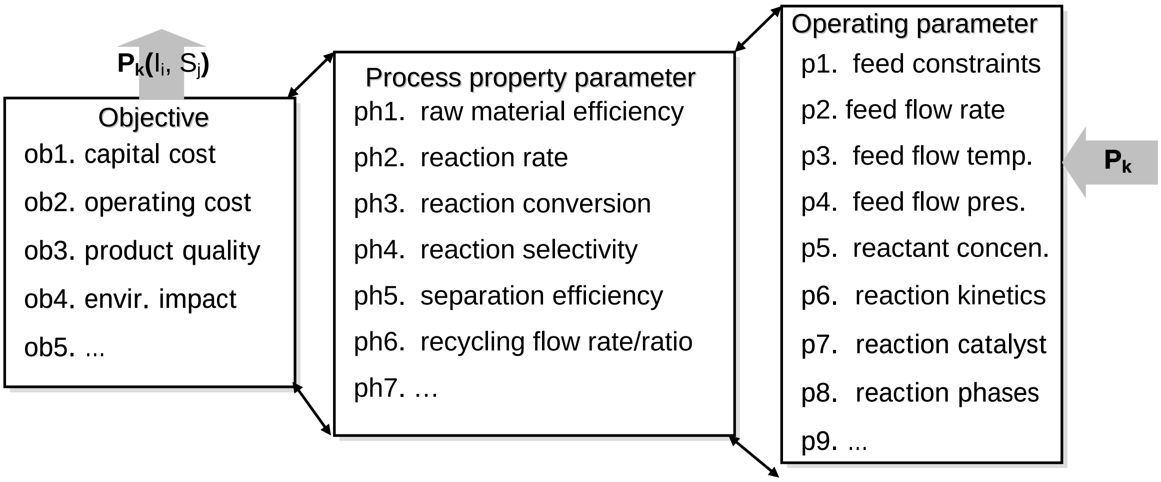


Fig. 14. The parameters of building RS conflict table.

Step 4: analyse and group the design heuristics via the conflict-based model.

When applying the design heuristics, the changed operating parameter will bring out the conflicts among the process properties. This results in a changing relationship between the objectives concerned. Therefore the implicit information is extracted from the design heuristics. The indicators could be used to express the influence of the applied heuristics to the characteristics. Then group the design knowledge and heuristics which have a contribution to the same conflicts among the characteristics identified.

Take heuristic 2 as an example: when applying the excess of reactants, the feed flow rate is increased. It improves the reaction rate while the raw material efficiency is getting worse. There occurs the conflict among those two process properties. Consequently, this has the positive affect for capital cost but not for operating cost. Indicator I_3=3, which indicates the applied heuristics will improve the objective in the cell of left column but decrease the one in the cell of the top row, is used to describe the relationship between the affected objectives. It is clear the heuristic is applied to the region of input in the flowsheet structure S_1. Therefore, heuristic 2, together with the identified indicators $P2(3,S_1)$, is arranged into the intersectional cell of the ones filled by studied objectives.

Step 5: formulate the conflict table by filling the grouped design heuristics into the table cells corresponding to the concerned characteristics.

As a result, the RS conflict table concerning multiple objectives is formulated.

4.4 Essential Features of the Methodology

The conflict-based method presents a new paradigm for representing and solving process synthesis and design problems. Compared with existing methods, the conflict-based method, as a knowledge-based method, decomposes the design tasks into groups of conflicts instead of existing hierarchical design levels (Douglas, 1988). The design problem is represented through the conflicts among the interrelated design objectives or the characteristics of the process. It highlights the consideration of the interconnections of the hierarchical design levels. There are several essential features of the proposed methodology.

Firstly, from the knowledge organization, the conflict-based model identifies the characteristics of certain chemical process domains; and reorganizes the available heuristics on the basis of their influence on the related process characteristics (objectives, process properties and parameters). It overcomes limited decision-making due to insufficient problem representation. It can assist the designers or users to understand the design problem in all its aspects, and also keep all available principles in mind for the problems under consideration.

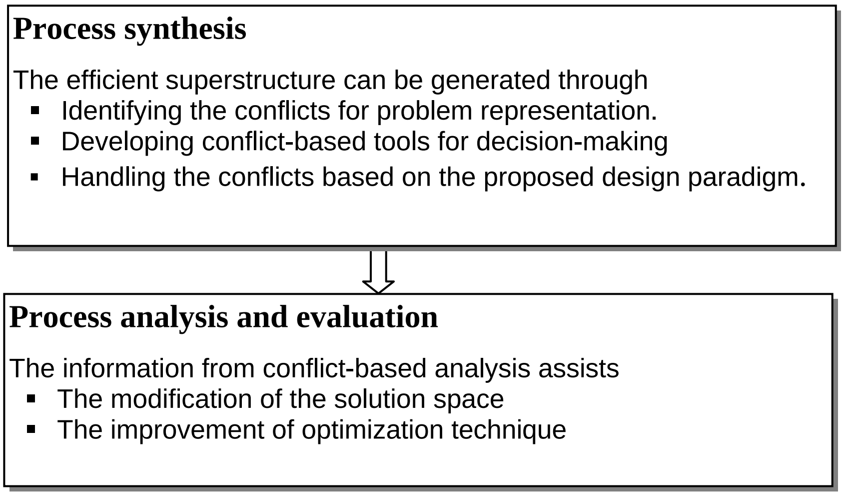
Secondly, from the point of view of methodology development, the conflict-based method presents a new strategy of evolving conflicts to carry out the design process. The conflicts among the objectives are transferred to ones among the process properties and operating parameters. The problem representation supports the systematic solving of design problems. The conflict-based method, based on selecting the design heuristics through the conflict table, exemplifies the generation of promising alternatives and innovative alternatives at the early stage of process design.

Thirdly, in the problem solving, the proposed approach combines conflict-based analysis in the early stage design and process analysis and evaluation in the detailed design stage. Conflict-based analysis is applied at the early design stage for screening and evaluating process alternatives. The generated process alternatives consist of an efficient and compact solutions space for the detailed design stage, where a quantitative technique is applied for optimal process alternatives. The conflict-based method minimizes the number of conflicts during the early design process by considering the multi-objective requirements. It reduces the complexity and conflicting nature of the design problem to support the detailed optimization stage, through considering only relevant design options without sacrificing optimality among all potential options. It offers a systematic way of accessing promising process alternatives.

5 CASE STUDY

5.1 Overview of Case Study

This section illustrates the application to the conflict-based method for process synthesis. The main contribution of the case study lies in two aspects shown in Figure 15. Both aspects illustrate that the conflict-based method has important potential for facilitating the generation of efficient solutions in the detailed design stage. Firstly, the case study shows that the conflict-based method can systematically generate promising design alternatives or an efficient superstructure. The problem formulation addresses the process synthesis problems in the specific domain. The conflict tables are built as the design tool. The case study applies the proposed conflict-based paradigm and conflict table to evolve promising design alternatives. This could overcome the drawback of missing or redundant solution alternatives through applying enumeration or generalization of existing methods. Secondly, the case study shows the strategies, based on the information gained from the conflict-based analysis, which could be explored to bridge the gap between the application of qualitative knowledge and quantitative techniques. It shows that applying the extracted information could reduce the optimization computational load and improve optimization techniques.



Process synthesis

The efficient superstructure can be generated through

- Identifying the conflicts for problem representation.
- Developing conflict-based tools for decision-making
- Handling the conflicts based on the proposed design paradigm.

Process analysis and evaluation

The information from conflict-based analysis assists

- The modification of the solution space
- The improvement of optimization technique

Fig. 15. The contribution of the case study

5.2 Process Synthesis (IV, V, VI)

Three problem domains are studied for the development of the methodology. They involve reactor/separator systems, distillation systems and waste minimization. The motivation for choosing these domains is based on the fact that a great deal of design heuristics and experiences exist in these fields. The design knowledge could be extracted from available books and publications and it is proved to be critical for the conceptual process design. Therefore, for the cases studied, the design knowledge is reorganized in order to apply the concept of conflict and to build the conflict-based tools to evolve the design methodology. The general procedure of the case study is carried out along the proposed design paradigm illustrated in Figure 16. The following sections show the motivation, the implementation of the design concepts and the results for the cases under consideration. The detailed study of three cases is presented individually in papers **IV**, **V** and **VI**.

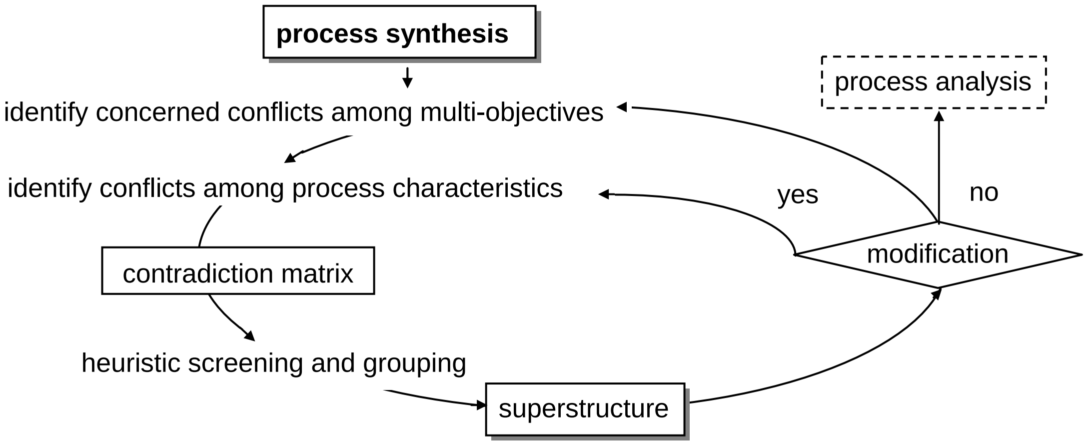


Fig. 16. The general procedure of process synthesis

5.2.1 Reactor/Separator System Design (IV)

5.2.1.1 Problem formulation

Processes synthesis of reactor and separator (RS) systems is one of the important tasks of chemical process design. The synthesis of a RS system relies heavily upon an efficient reaction-separation superstructure. Due to the complex structure interconnection and the multi-objective design requirements, the issue of how to build a highly-representative superstructure is of critical importance. Much work has been done to address this problem. Floquet et al. (1985) proposed a tree searching algorithm for the reactor/separator sequence synthesis. Fredler et al. (1993) introduced a graph theory approach that has polynomial complexity to find all the interconnections in process networks. Nisoli et al. (1997) combined the attainable region approach for reactor synthesis with geometric concepts of feasibility of separation. However the issue of process synthesis for the fulfilment of the multi-objective requirement and integrated phenomena of reaction and separation is not addressed by existing methods in the generation of the superstructure.

It is observed that very often different conflicts and contradictions occur when addressing the multi-objective issue in the generation of the superstructure. The problems emerged are usually handled by trade-offs during the early design stage. This may result in missing promising alternatives, unsatisfactory fulfilment of the design objectives or in the formulation of hard-to-solve mathematical problems. Therefore the aim of applying the conflict-based approach is to generate highly representative superstructures with regard to the multi-objective nature of the process design.

5.2.1.2 Methodology development

The conflict table for the RS system is built and the phenomena-relationship graph is constructed for the RS system. For the given specific problem, the specific phenomena-relationship structure can be identified based on the constraints and specification of streams and processes. It is the basis of superstructure generation. Based on the abstraction of the phenomena-relationship structure and the application of conflict tools, the superstructure is systematically generated by the conflict-based method taking into account the multi-objective nature of the design process.

Conflict table for reactor/separator system:

The RS conflict table is built to deal with the multi-objective conflicts. It is composed of 8 design objectives, such as capital cost, product quality, environmental impact, and 86 extracted design principles for the synthesis of RS system from available literature (Douglas, 1988 and Smith, 1995). The design objectives form the rows and columns of the matrix and the design principles P_k (I_i, S_j) constitute the matrix elements as shown in Table 2. The design principles P_k, k= 1-86 are extracted based on the available literature (Douglas, 1988 and Smith, 1995). Every principle is characterised by a so-called influence coefficient $I_{i,}$ (I_1=1,

I_2=2, I_3=3, I_4=4) and flowsheet phenomena indicator S_j (j= 1-5). The influence coefficient I_i represents the character of the influence on the two concerned objectives when applying the principle; e.g. if the application of the given principle will improve both objectives then use I_1. If the application of the given principle will worsen both objectives then use I_2. And finally, if the application of the given principle will improve one objective but worsen the other then use I_3 or I_4. The flowsheet phenomena correspond to the region of the flowsheet structure in which the given principle should be applied; e.g. S_1=feed, S_2= reaction, etc.

Table 2. A fragment of the reactor/separator conflict table

	1.captial cost	**2.operation cost**	**3.product quality**	**4.environ. impact**	**5.safety**	**6.complexity**	**7.flexibility**	**8.controllability**
1	**	p2 (3, S1) ...	p1(1,s3) ...	p4(4,s4) ...	p58(4,s3) ...	p22(4,s3) ...	**	p11(4, s3) ...
2		**	p4(4,s4) ...	p6(4,s3) ...	p8(4,s3) ...	p22(1,s3) ...	**	p14(3,s3) ...
3			**	p1(1,s3) ...	p33(3, s4) ...	p23(1, s3) ...	p31(1, s4) ...	p12(3, s3) ...
4				**	p8(3, s3) ...	p28(2, s4) ...	**	p48(3, s3) ...

The RS conflict table reorganizes the available design principles based on their possible influence on the design objectives. The design principles are activated if the influence coefficient is I_1, I_3 or I_4 as well as the correlated process phenomena. The selected principles are screened using the RS matrix. The full RS conflict table and the heuristics, which are modified based on the previous version applied at attached papers, are given in Appendix **I** (Table 1 and 2). The guidewords and extracted process parameters for the heuristic study are listed in Appendix **I** (Table 3 and 4). The design principles are used to evolve the superstructure and to analyse the potential optimal structure for the particular objectives.

5.2.1.3 Phenomena relationship structure

Based on the generic phenomena structure as proposed in section 4, the phenomena-relationship graph for a RS system is proposed. Here the phenomena mean the process phenomena rather than the thermodynamic phenomena. They include the transport phenomena and transform phenomena as shown in Figure 17.

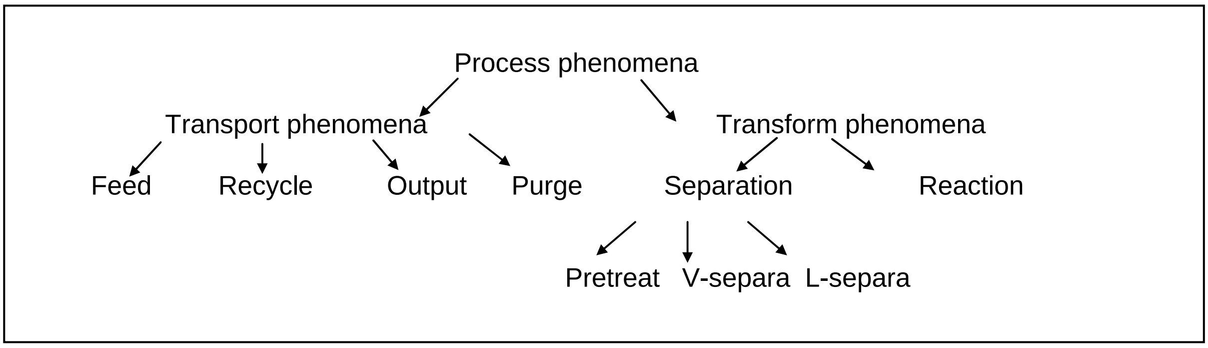


Fig. 17. The process phenomena

There is a general flow pattern among the process phenomena for every stream. On the one hand, the general flow pattern caters to all different flowsheet configurations without considering the number of units and their types; on the other hand, it shows the possible locations of phenomena integration. The phenomena-relationship graph consists of two parts as shown in Figure 18: one is the phenomena interconnection graph that shows all the possible connections among the phenomena; the other gives phenomena integration points which indicate possible locations of process integration, such as a combination of reaction-separation phenomena and complex distillation systems.

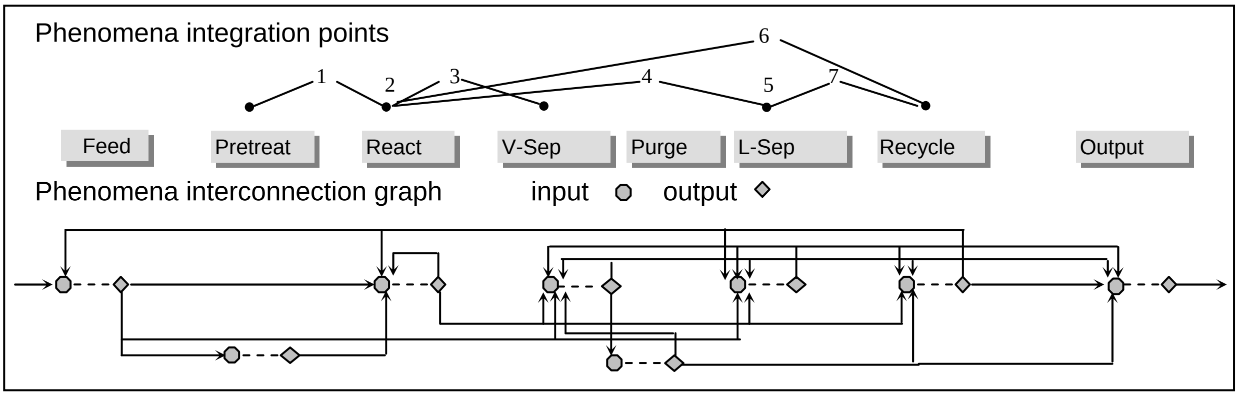


Fig. 18. The general phenomena-relationship graph

5.2.1.4 Case implementation

The proposed approach is illustrated with the synthesis of the hydrodealkylation of toluene (HDA) process. The HDA process has been extensively studied by Douglas (1988) applying a hierarchical heuristic synthesis approach. In this case study, problems involved consist of the systematic generation of a highly-representative flowsheet superstructure, the identification of the promising flowsheet configuration and some of the operating conditions based on multi-objective requirements.

The proposed design paradigm of the conflict-based method is realized by a three-step procedure for the synthesis of RS networks. In the first step, the phenomena-relationship structure is extracted from the proposed general structure of all potential interconnections among the anticipated phenomena. The basic configuration is formulated under consideration of the specific process streams. At the second level, the design objectives are identified and conflicts between them are analysed. Based on the specification of the process, five concerned objectives are identified: capital cost (1), operational cost (2), product quality (3), environmental impact (4), and controllability (8). Sequentially 10 conflicts are formulated among them, such as conflicts between capital cost and operation cost (1 x 2), capital cost and product quality (1 x 3), environmental impact and controllability (3 x 8), etc. The design principles are selected for removing these conflicts and grouped into phenomena blocks via the so-called RS conflict table. Applying the selected principles together with the design specifications, a flowsheet superstructure is generated on the basis of the phenomena-relationship structure. Then optimization is carried out for searching for the optimal synthesis solution. The details can be found in paper **IV**.

The work is based on objective conflicts driven problem solving, allowing the generation of the promising alternatives with their emphasis effects of the design objectives. The approach also benefits from the presentation of the process flowsheet, allowing for determination of plant wide connectivity and initial ranges of values for ‘optimization variables’, without requiring the formulation of a rich superstructure consisting of numerous interconnected unit operations.

5.2.2 Distillation System Design (V)

5.2.2.1 Problem formulation

Due to its wide use in process industry, studies on the design of distillation processes are still challenging. Distillation is the largest energy consumer of all chemical operation units. Thus the design of energy efficient distillation processes is always one of the objectives of design problems. The knowledge-based approach is a widely studied method for the design of distillation-based processes. Despite the fact that there are many heuristics for the sequencing of distillation trains for multi-component mixtures, it is still difficult for designers to use those heuristics to solve practical problems due to their conflicted influence on the multi-objectives. Therefore there is still no systematic method for distillation-based process design which considers all possible heat integrated strategies and the process background (Smith 1988, Gundersen 1991).

To obtain an optimal distillation process, the following hierarchical issues should be considered.

- Synthesis of simple column sequences.
- Synthesis of heat integrated distillation flowsheet through heat matching among simple columns.
- Synthesis of complex distillation flowsheet.
- Synthesis of distillation flowsheets considering simultaneously complex columns and heat integration.
- Synthesis of distillation flowsheets considering its background process.

Therefore, synthesis of a distillation process is a combinatorial and hierarchical problem. It is difficult to consider or combine all these problem levels during the synthesis process. Since all these problems are based on common process properties and parameters, it is promising to develop conflict-based tools to extract common process characteristics, to analysis the conflicts among them, and to handle the conflicts via the application of design heuristics. The conflict-based method is applied for the synthesis of the distillation system. The specific conflict table is constructed. However, the developed conflict table is not intended to provide an automatic implementation of distillation process design. The goal here is to point out the possible decision-making for process design. The main purpose of the conflict-based method is to support designers to make the right decisions towards the optimal design.

5.2.2.2 Methodology development

For the distillation system, the conflict table is built based on 31 characteristics and 29 principles through literature study and expert experience (Rong et al., 2000). The 31 characteristics represent the distillation flowsheets' physical states and the performance of the distillation flowsheets. The principles are used to justify decision-making for design improvement of distillation flowsheet, including 20 specific principles and 9 general principles. These principles extend the alternative space automatically from traditional distillation schemes to non-traditional ones. Based on the identified characteristics and principles, a conflict matrix is built.

Table 3 shows part of the conflict table for distillation systems (Rong et al., 2000). When improving the characteristics listed at the cells of left column, it may worse the ones shown on the top row. There occur conflicts among the process characteristics, which are handled by the related principles. The indexes of those principles are listed at the intersectional cell of the ones filled by the studied characteristics. The order of applying principles in the singular cell is case-oriented based on process knowledge and expert experience.

Table 3. A fragment of the conflict table for distillation systems

CHARACTERISTICS		**Characteristics that are getting worse**						**PRINCIPLES**	
		…	23	24	25	26	…		
1	feed condition		23,22 24,25	7,1,2,9 20,15	4,1,2,3 16-20	10,11 12,3,5		changing method	1
… 16	heat exchanger number.		22,24	9,20,7	4, 16-20	11,10 12		intermediate heat exchanging	… 16
17 …	compressor number		23,25	4,6,8 17,20	4,7,6 16-20	12,11 10		heat matching among columns	17 …
23 …	complexity		***	9,15, 13	1,3, 2,4	12,11 25		balancing the role of computer and human	29

The characteristics help the designers to fully understand all aspects of the distillation problems. Moreover, all available principles allow the generation of nearly optimal alternatives. It can overcome the limitation of incorrect decision-making due to insufficient knowledge and psychological inertia of designers and engineers. In particular, it allows designers to consider all heat-integrated strategies through examination of all characteristics and careful consideration of the principles of the distillation systems design. The complete table is given in Appendix **II**, which consists of the conflict table of design objectives, of process characteristics, and of objectives to process characteristics.

Characteristics of distillation processes:

The characteristics of distillation processes are identified as presented in Table 4. The characteristics or parameters are used to describe the physical states and performance of distillation flowsheets. There are 23 distillation process characteristics and 8 objective attributes are considered.

Table 4. Characteristics of distillation process

Process characteristics:
1. feed conditions
2. separation specifications (products and purifications)
3. constraints of components in the mixtures
4. type of separation agent
5. relative volatilities
6. reflux ratios
7. number of trays
8. amount and composition of purges (gas, liquid)
9. temperature profile
10. pressure profile
11. energy flow profile
12. mass flow profile
13. number and types of distillation columns
14. number of condensers
15. number of reboilers
16. number and types of heat exchangers (include cooler and heater)
17. number and type of compressors
18. hot utility levels of a system

19. cold utility levels of a system
20. number of recycle streams in a system
21. number of purge streams in a system
22. uncertainties of a system
23. complexity of a system

Objective characteristics:

24. capital cost
25. operating cost
26. environment impact
27. safety & relief
28. flexibility
29. controllability
30. capacity and productivity
31. lifetime cycle (development, design, operation, maintenance, disposal…)

Principles for distillation process design:

Since the distillation process is a multi-level decision-making problem, specific design knowledge or heuristics exists to aid the decision-making, such as for the synthesis of simple column sequences. However, there is a lack of detailed knowledge for certain problems, like how to deal with the uncertainty of the system. The solutions are quite situation-based. Therefore design principles have been extracted which involve specific suggestions (Table 5) for the designers to perform a specific activity; and also some generic guidance (Table 6) to lead the decision-making in the right direction. All principles here aim to improve the performance of the distillation flowsheet from the point of view of process synthesis, especially the aspect of heat integration, which is an important aspect in improving the performance of distillation processes. It involves many strategies and concepts such as side-stream columns, intermediate heat exchanging, and heat matching among simple columns, pump distillation schemes, multi-effect distillation schemes and thermally coupled schemes. They are all generalized as principles for improving the performance of the distillation flowsheet.

Table 5. Specific principles for distillation process design

1. change separation method
2. change the component (product) separation sequence
3. change the separation agent (for mass separation agent based methods)
4. heat integration principle
5. mass integration principle
6. change the temperature and pressure of separators
7. change the reflux ratio of column
8. change the number of trays of column
9. consider the use of multifunctional units
10. change the number of recycle streams, their recycle flow rates and compositions.
11. change the interconnections between the units
12. change the steams' compositions
13. increase or decrease the number of units in a system
14. change the utility levels to match the heat flow profile of a system
15. consider a complex distillation scheme with side stream column
16. consider heat integration strategy of intermediate heat exchanging
17. consider heat integration strategy of heat matching among simple columns
18. consider heat integration strategy of heat pump distillation schemes
19. consider heat integration strategy of multi-effect distillation schemes
20. consider heat integration strategy of thermally coupled distillation schemes

Table 6. The general principles for distillation process design

21. bottlenecks identified first principle
22. decomposition and independence principle
23. design process following the evolution from simple column to complex column
24. simplification principle (complexity reduction principle)
25. considering and understanding the sequential and hierarchical nature of process design
26. combination of qualitative and quantitative information principle
27. knowledge and experience maximize utilization principle
28. information content balance principle
29. balancing the role of computer and human principle

5.2.2.3 Case study

The retrofitting of an existing industrial complex distillation process of a butadiene extractive distillation plant is studied by the conflict-based method. The aim of the design is to improve the process flowsheet to satisfy multi-objective requirements. This case was selected because it involves the various types of distillation columns; moreover, the process is energy intensive feature and improvements in environmental impact are possible. The case study follows the proposed design paradigm: the three-levels design procedure. First, the conflicts among the objectives are analysed to identify the sub design task or major structural issues which are essential for trading-off the objective conflicts; Next, the sub design tasks are represented by the identification of the conflicts among the process characteristics. They are solved by using conflict-based design tools and thermodynamic analysis. As a result, promising flowsheet alternatives are generated which are subject to evaluation in the third step, simulation or optimization. This procedure is iterated until no further improvements to the flowsheet can be made.

Four general objective conflicts, such as lower operating and capital cost, solvent choice and environmental issues, lower operating cost and lower flowsheet complexity etc, are considered at the first level. When using the appropriate principles to remove these general contradictions, the essential sub design tasks are identified which involve the solvent evaluation, heat exchanger network and process integration. Then twelve further contradictions among the process characteristics are identified at the consecutive level. With the thermodynamic analysis, the contradictions in the lowest level are identified for the final debottlenecking and optimization. As a result, the possibilities for the use of feasible heat-integration strategies and complex distillation schemes are explored for this retrofitting problem. Correspondingly the conflict-based method for problem solving is examined by searching for the optimal retrofitting solution. The details can be found in Paper **V**.

5.2.3 Waste Minimization Design (VI)

5.2.3.1 Problem formulation

As a result of increasing public pressure and more restrictive regulations, waste treatment has become a more and more important issue for chemical process synthesis. The traditional end-of-pipe treatment approach, which aimed to eliminate the pollution generated, is not an efficient method from the point of view of sustainable development. Current research efforts pay attention to the reduction of waste sources using a hierarchical approach, such as the Douglas hierarchical procedure (Douglas, 1992) and onion diagram (Smith, 1995). Waste minimization is, however, a complex decision task that involves waste handling and multi-objective analysis.

Waste treatment always generates conflicts among the design objectives. These contradictions cannot be handled in a satisfactory way using existing hierarchical decision-making methods. Therefore it is promising to apply the conflict-based method to deal with the contradictions arising during the design of the processes.

5.2.3.2 Methodology development

Conflict table for waste minimization:

A matrix of waste minimization is formulated based on 12 extracted characteristics and 31 heuristics and techniques of waste minimization. The knowledge reorganization is based on analysis of the heuristics and techniques that improve the characteristics related to the waste sources and their contributions to the process design objectives. Twelve dominant parameters for identification of the sources of waste minimization are extracted as listed in Table 7. The following objectives are considered in this matrix: economic criteria, product quality, safety and controllability. Every objective is composed of its sub-objectives, which are listed in Table 8 (Douglas, 1988). Heuristics is selected based on Halim et.al. (2002) and Dantus et.al. (1996). The details of the heuristics are listed in Table 9. The heuristics are divided into four groups that deal with changes in the product, transformation of input material, modifications of technology and good manufacturing practice.

Table 7. Identified parameters of waste reduction sources

1. raw material conditions	7. recycle ratio
2. raw material efficiency	8. purge or emission ratio
3. reaction conversion	9. side product treatments
4. reaction selectivity	10. product specifications
5. separation solvent	11. heat efficiency
6. separation efficiency	12. process configuration

Table 8. Design objectives concerned

1. Economic	1.raw material cost	2. equipment cost
	3. utility cost	4. product profit
	5. start-up cost	
2. Product quality	1.product species	2. product amount
	3. product purity	
3. Safety	1.ionising risk	2.explosion risk
	3. toxicity risk	4. high T/P risk
4. Controllability	1. operating condition	2. process flow control
	3. recycle control	4. unit operability

Table 9. The heuristics for waste minimization

Product change		
1. product substitution	2. product conservation	3. change product composition
Source reduction		
4. material purification	5. material substitution	6. raw material updating quality
7. process changes	8. equipment, piping, layout change	9. additional information
10.changes in operational settings	11.prevent useful excessive feed	12.increase the conversion
13. change type/configuration of reactor.	14.optimize reactor or operating conditions to eliminate or reduce generation of waste material	15.choice of suitable separation solvent
16.suitable separation method	17. separation unit sequence	18. separation unit structure
19.heat integration	20. process integration	21. purify purge/emission stream by additional purification system
Recycling		
22. use or reuse by recycling the useful material to original process	23.raw material substitute for another process	24.reclamation: processed for resource recovery
25. processed as by-product		
Good operating practices		
26.procedural measures	27. loss prevention	28. management practices
29. waste stream segregation	30. material handling improvement	31. production scheduling

Every heuristics is placed into the intersectional cell between the characteristics concerned and the design objectives influenced as shown in Table 10. The symbols ‘+ -’ are assigned to the available heuristics. The symbol ‘+’ means that the process objective concerned is improved when applying the heuristics; ‘-’ means its deterioration. The symbol indicates that the application of the heuristics for waste minimization results in changing the values of different objectives. This may lead to conflicts among the objectives concerned. Therefore, via this matrix, suitable heuristics of waste minimization can be evaluated and selected based on analysing the conflicts among the process objectives. The full matrix is given in Appendix **III**.

Table 10. A fragment of the conflict table for waste minimization

Characteristic of WM	**Design Objectives**											
	E1	…	E5	Q1	…	Q3	S1	…	S4	C1	…	C4
1	H6(+)					H4(+) H5(+)				H6(-)		
2	H11(+) H22(+)		H11(-) H30(-)		H22(+)	H30(+)					H22(-)	

Two meta-heuristics are identified to select the heuristics of waste minimization as below. They support the conflict-based analysis among the multi-objectives.

- Selecting the heuristics having a positive influence ‘+’ on the design objectives concerned and screening out the heuristics which have a negative effect ‘-’ on the design objectives.
- Trading off the heuristics having simultaneously positive and negative influences on various design objectives.

Based on the objective-oriented analysis of the heuristics, the alternatives for pollution prevention are evaluated and refined. Moreover, the potentially optimal structures from the point of view of the particular objectives are indicated by the analysis of the respective objectives.

5.2.3.3 Case study

A case study, an air-based direct oxidation process for the production of ethylene oxide, is presented for illustration of the proposed approach. A step-by-step systematic approach is proposed to ensure the reduction or elimination of the conflicts with regards to waste handling and multi-objective synthesis. Pollution prevention alternatives are identified and the superstructure aimed at waste minimization is formulated for further mathematical optimization.

In the first step, the base case is used to evaluate the current performance of the process and to detect the characteristics that are related with the waste sources. Five key parameters are identified to reduce waste sources: the raw material conditions, reaction conversion, separation efficiency, purge or emission ratio, and heat utility efficiency. Next, in order to improve these characteristics, the developed matrix is used for selecting the suitable heuristics or techniques which ensure the reduction or elimination of the conflicts with regard to waste handling and multi-objective synthesis. Then, pollution prevention alternatives are identified. Together with the base case, the superstructure aimed at waste minimization is formulated. The superstructure is modified and verified by checking the identified key parameters of waste sources and repeating conflict-based analysis. It is shown that the superstructure aimed at waste minimization can be systematically formulated using the conflict-based method. The detailed case study can be found in paper **VI**.

5.3 Process Analysis and Evaluation (VII, VIII)

The work in this section shows that the results and information derived from the conflict-based method can support the detailed design stage. Their contributions lie in the modification of the solution space and the optimization technique. It examines that the conflict-based method could provide information to bridge the gap between the application of qualitative knowledge and quantitative techniques. It has considerable potential for facilitating the generation of efficient solutions at the stage of mathematical optimization.

The flowsheet superstructure is systematically generated via the conflict-based method as explained in the above section. On the one hand, the conflict model transfers the design task from objective levels to the parameter level; on the other hand, the conflict table visualizes the contribution of the various heuristics to the different design objectives. The various heuristics correspond to the various operating parameters and flowsheet structure of the generated superstructure. It provides potential information together with the evolving of the superstructure. For example, the weights of importance of the operating parameters to the design objective, and the weights distributions of the various structures corresponding to the multi-objectives. This information can be extracted and used for modification of the solution space or optimization technique to assist the next stage of process optimization as shown in Figure 19.

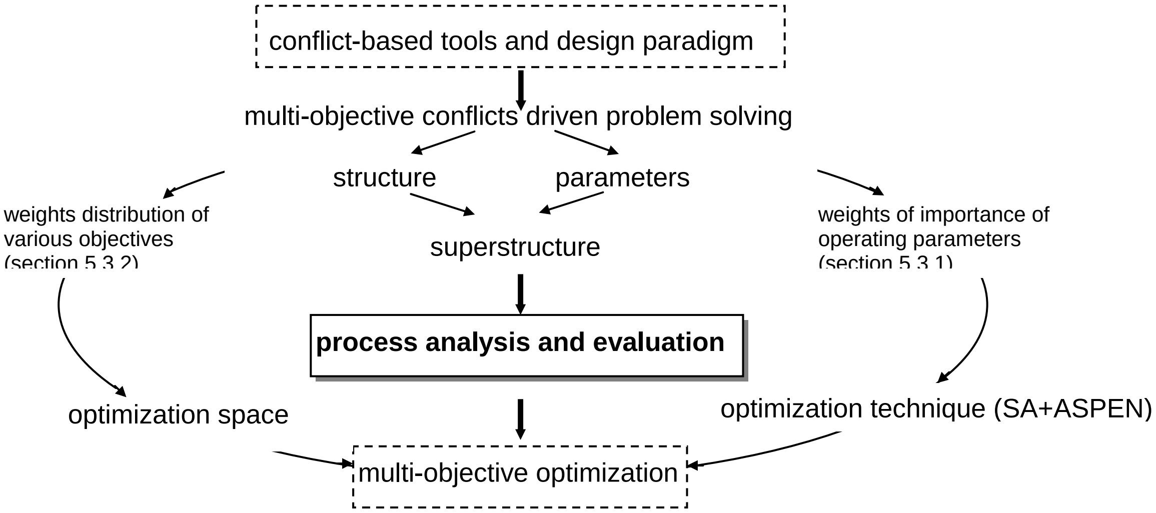


Fig. 19. Framework for process analysis and evaluation

5.3.1 Improvement of Optimization Technique

The conflict-based method assists the generation of the superstructure at the early design stage. Then a simulation based optimization framework is proposed for searching for final optimal solutions. The Simulated Annealing (SA) algorithm with ASPEN simulator is applied as the multi-objective optimization technique. The method of summation of weighted objective functions is used to convert the normalized multi-objectives function into one utility function.

The SA technique optimises the configuration through the evolution of the structural and stream states. However it is very computationally demanding to get the Pareto set for each possible configuration. A strategy is proposed for modifying the SA algorithm by dynamically adjusted stepsize (DAS) for continuous variables. It is established on the work of step width adaptation done by Nolle et al. (2001). DAS speeds up the solution search by adapting the changed stepsize to the current iteration. It is based on consideration of the importance of the variables for the optimization target or objectives. The information is extracted from the conflict-based analysis in early stage. To optimise the continuous variables, SA adapts the DAS to current iteration. The efficiency of the method is measured by the number of the function evaluation and CPU calculation time of every obtained Pareto point.

The HDA process has been studied to examine the proposed strategy. The problems presented here consist in the conflict analysis between economic criteria and environmental impact for screening and evaluation of process alternatives; and optimization of the alternatives by modified simulated annealing with a process simulator. Multi-objective optimization takes into account the trade-off of the conflicts between the economic criteria and environmental impact. The first objective seeks to minimize the negative profit (-P). The evaluation of environmental impact is based on the waste reduction (WAR) algorithm (Cabezas et al., 1999).

The optimization results suggest that the proposed strategies can improve the computational efficiency while keeping optimization accuracy. It proves that the information, derived from the conflict-based method, can be used to improve the optimization technique for the following optimization process. Then it can bridge the gap between early qualitative information and detailed optimization techniques. Details of the work can be seen in paper **VII**.

5.3.2 Modification of the Solutions Space

Conflict-based analysis in the early design stage is aimed at evolving and screening process alternatives via the conflict table. The matrix is used to identify the conflicts between the design objectives and to select useful principles for removing the conflicts. The qualitative reasoning method is applied for evaluating the heuristics and handling uncertain design knowledge. It is based on the contribution of the applied heuristics to the objectives concerned. As the result, the heuristics are evaluated and the relevant insights concerning the relationships between them and the corresponding objectives are discovered. This enables the formulation of a high-representative superstructure with valuable information with regard to the multi-objective nature of the design. It efficiently supports the next step, multi-objective optimization.

The qualitative reasoning method, evidential reasoning approach, is adapted for evaluating the design heuristics under the consideration of the multi-objective requirements. The input qualitative information is the evaluation grades together with the confidence degree. The former item represents the relative contributions of the heuristics to the sub objectives; and the latter one means the degree of subjective uncertainties when applying the heuristics (Sen et al., 1998). The method applies the evidence combination rule of the Dempster-Shafer theory, which is a powerful tools to deal with uncertainty. It has been proven that it is an efficient method capable of dealing with incomplete, qualitative information in a more rational way than other tools (Yang et al., 1994). The TOPSIS method is adapted for ranking and comparing the evaluation results. Details of the reasoning method can be found in the paper (Yang et al., 1994).

The heuristics is evaluated which corresponds to the multi-objective criteria based on the qualitative reasoning. Furthermore, the degree of their contribution to the objectives concerned, that is, the weights distribution of the objectives, is refined by identifying the so-called dead zone. The identification of the dead zone can significantly improve the calculation efficiency of the next optimization through reduction of the sampling number in this weight range. Therefore, the optimization space is refined and the combinational size of the synthesis problem is significantly reduced to improve the computational efficiency of stochastic optimization techniques. Moreover, it assists in the generation of an evenly distributed Pareto set via the refined weight range.

Case study of HDA process synthesis and optimization is used to illustrate the proposed method. It shows that process analysis, on the basis of the results of the conflict-based method, is able to bridge the gap between early decision-making and detailed process optimization through evaluating and screening process alternatives. The solution space is modified to efficiently support a rigorous optimization process. Details of the case study can be referred to the paper **VIII**.

6 SUMMARY

6.1 Contributions

The thesis presents the development of conflict-based methodology for process synthesis. It is towards the way of enabling the fulfilment of the multi-objective requirements and the enhancement of the creativity of design activities. The contribution of the work involves the following aspects:

1. Understanding CPS using the concept of conflict.

The problem studied is conceptual process synthesis of chemical processes. In order to enhance the creativity of design activities, a new design concept has to be chosen and applied to developing design methodology. The conflict model is proposed for presenting the design problem at a conceptual level.

2. Developing the conflict table and design strategies to support decision-making.

Design tools are formulated based on the new concept. It reorganizes the available design heuristics and experiences of a certain problem domain. The information is used to support decision-making in conceptual process synthesis. Problem solving strategies are concluded to guide the design activities towards a way of searching for optimal solutions.

3. Formulating the conflict-based design paradigm for CPS.

A general design paradigm is proposed for supporting process decision-making in the presence of multi-objectives and an uncertain environment. The class of problem is formulated into a conflict-based decision process that incorporates multi-objective requirements. Based on the conflict-based analysis, the achieved results and information can be used to bridge the gap between qualitative and quantitative knowledge through the explored algorithms. A simulation based optimization framework is proposed to solve the synthesis and design problem.

4. Demonstrating the applications of the developed method to specific process systems.

Applications are investigated that involve hierarchical decisions and multiple conflicting goals, e.g., economic criteria and environmental impact, in which the decision makers ought to maximize expected profit while minimizing environmental impact. The application domain involves reactor/separator systems, distillation systems and waste minimization. The motivation of choosing these problem domains is based on the fact that a great deal of design heuristics and experiences exist for these domains. The methodology developed is evolved and implemented through case studies.

6.2 Remarks

The work is based on a new concept and design paradigm adapted from TRIZ methodology. TRIZ is claimed to be a ‘systematic creativity’ framework thanks to its knowledge function delivery and trends of evolutionary tools (Mann, 2002). Enhancing creativity is carried out through the systematic way of identifying problem solving opportunities. These are the foundation of developing the conflict-based method for process synthesis to deal with its combinatorially complex characteristics and evolutionary nature. It is claimed that the concepts and activities of process synthesis can be modelled and creativity can be simultaneously supported.

The developed methodology reflects the conflict nature of process design and synthesis. The conflict-based model aims to represent the design problem in the hierarchy of the conflicts of the design objectives and process characteristics (process properties and operating parameters). Evolving the conflicts from the level of conflicts among the objectives to the level of the conflicts among the process characteristics realizes the task of decomposition and reflects the evolutionary nature of the design process. The level of conflicts among process properties is a combination of the process operating parameters. Furthermore, they are the characteristics of process phenomena such as reaction, separation and recycle. These conflicts carry out the function delivery between the conflict levels of objectives and operation parameters. Handling these conflicts, on the one hand, reduces the function complexity between the design objectives and the operating parameters, and on the other hand, overcomes the limitation of the boundaries of traditional unit operations. The conflict-based representation reduces the complexity and combinational nature of the design problem by considering only relevant design tasks. It assists the design targeting and problem debottlenecking of process synthesis.

The conflict-based tools are built by identifying the characteristics of the process and extracting the available design knowledge and heuristics. The tools can assist designers or users to comprehend the design problems in all its aspects, and also keep all available principles in mind for the problems at hand. The organization of the design heuristics and experience is constructed according to their contribution to the abstract levels of the conflict model. The selection or the screen of the heuristics is based on the strategies of identifying uncoupled conflicts and minimizing the number of conflicts at an early stage of design. This can facilitate design activity in the detailed design stage.

A combined design paradigm is proposed for handling multi-objective conflicts of process synthesis in both the early and detailed design stages. It bridges the gap between the design activities of the early design stage and those of the detailed design stage. The conflict-based tools are used for screening and evaluating the alternatives to evolve the process superstructure. An efficient and compact solution space built at the early design stage can improve the efficiency of simulation and optimization in the detailed stage. It can overcome the drawback of missing or redundant solution alternatives by applying enumeration or generalization of existing methods. Strategies to bridge the gap between the application of qualitative knowledge and quantitative techniques are also explored.

To conclude, this work develops the conflict-based method to support decision-making of design and to handle its multi-objective requirements and combinatorially complex nature. The design concept and paradigm are implemented and validated through case studies. The enhancement of the creativity of design activities and the improvement of the engineering design practice are demonstrated through the systematic procedure of evolving possible design alternatives and searching for optimal solutions.

6.3 Discussion

Process design is a creative activity. Enhancing the creativity of design is becoming an essential part of the methodology of process R&D. The complexity of the design process presents many challenges in understanding and supporting creativity. TRIZ method highlights the contributions of generic design procedure, generalized system characteristics and principles, to the enhancement of creativity. It determines that TRIZ based method is aimed for exploring ideas and solutions at early design stage instead of providing deep process ‘know-how’. Then this method can be called rather an idea generator than a problem solver. Moreover, for chemical process synthesis and design, the deep design knowledge and specific process characteristics provide the important factors for improving the creativity of design activities. This challenges the direct application of TRIZ method for chemical process synthesis. Therefore, at this work, although it explores a generic design framework for chemical process synthesis, the studied design knowledge and developed tools are specific domain based. It limits the practical application of the developed method and tools for other issues of chemical process synthesis.

Due to the complexity and evolutionary nature of process design, conceptual design is always regarded as non-methodological. This puts limits on how process design is systematized and how ‘detailed’ a level is attainable. Although the work presents a systematic way for process synthesis, the developed tool or strategy itself does not directly select certain design heuristics and generate the promising process alternatives; it does, however, provide a systematic way of identifying the opportunities for problem solving. The designers, based on their knowledge and design specifications, need to decide how detailed the conflicts of the design targets should be, to name the next relevant level of the conflicts, and to select the suitable heuristics through the design tools.

The work organizes the information of a specific problem domain for building a conflict table. The conflict table is used as a design tool to support decision-making. The main idea here is identifying opportunities towards evolving promising alternatives rather than generating new design heuristics. The information analysis of design knowledge and heuristics is based on studies, understanding and discussion of the research team. Rather than developing an efficient knowledge based system, the aim of building the conflict table is to support the development of the framework of the methodology.

One of contributions of the proposed design paradigm is to bridge the gap between qualitative design knowledge at the early design stage and quantitative synthesis technique at the detailed stage. Based on information from the conflict-based analysis in the early design stage, the work explores strategies to modify the solution space and improve the optimization technique. However, the generality and systematisation of these strategies should be studied further.

Conflict-based method needs further development towards a way of automating process design. It involves those following issues.

- quantification of the conflict

The priority of various design tasks is important for effective decision-making. Since the design tasks are presented by the conflicts, the priority can be identified by quantifying the important degree of the conflicts at the same design level.

- quantification of the heuristics in view of the conflict concept.

The order of applying heuristics can be visualized through quantifying their contribution to the concerned conflicts. It supports the decision-making towards a way of searching optimal solutions.

- investigation of the algorithm for the problems solving strategies.

The detailed algorithm will be developed to implement the strategies of identifying independent conflicts and of minimizing the number of conflicts. Therefore the problem solving strategy could be carried out in a systematic and automatic way.

- development of the software to support the developed methodology and tools.

The computer-aided tools will assist the application of the methodology in academy research and industry.

The work presented in this thesis focuses on the framework and procedure of the methodology development. It should be noted that good features of a good process design methodology include the following two points: firstly, it should have the ability to integrate various design activities, such as process engineering, safety engineering, and more recently, product engineering; secondly, it should permit a natural way of incorporating the use of computers in decision-making, knowledge storage and retrieval. These features give perspectives for future research towards knowledge management and automation of process design. It is expected that the frameworks and methodology reported will be employed for other design cases and further research work.

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APPENDICES

APPENDIX I	Reactor/separator Conflict Table
APPENDIX II	Distillation System Conflict Table
APPENDIX III	Waste Minimization Conflict Table
APPENDIX IV- IX	Scientific Publications

I II III

Conflict table for
reactor/separator system,
distillation systems,
waste minimization.

APPENDIX I Reactor/separator Conflict Table

Table 1. Conflict table for reactor/separator system.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1. capital cost	**	P2 (3, s1) P4 (1, s4) P6 (4, s3) P10 (5, s3) P11 (5, s3) P15 (5, s3) P16 (1, s3) P17 (5, s3) P21 (4, s3) P44 (5, s3) P46 (5, s3) P47 (5, s4) P54 (4, s5) P58 (4, s4) P60 (3, s3) P63 (4, s2) P66 (4, s5) P67 (4, s5) P68 (4, s5) P75 (4 s5) P78 (4, s5) P81 (4, s5) P84 (4, s2) P85 (4, s3) P86 (4, s2)	P1 (1, s3) P3 (4, s1) P4 (3, s4) P5 (1, s3) P6 (4, s3) P7 (4, s2) P12 (4, s3) P14 (2, s3) P24 (3, s3) P46 (5, s3) P49 (4, s4) P55 (4, s5) P56 (4, s5) P59 (4, s3) P60 (1, s3) P63 (2, s2) P73 (4, s5) P74 (4, s5) P76 (4, s5)	P4 (4, s4) P6 (4, s3) P21 (4, s3) P28 (1, s4) P54 (4, s5) P56 (3, s5) P58 (4, s4) P59 (5, s3) P66 (4, s5) P71 (3, s4) P72 (3, s5) P75 (4 s5) P77 (1, s5) P78 (4, s5) P80 (3, s5) P81 (4, s5) P85 (3, s2) P86 (3, s3)	P58 (4, s3) P59 (4, s3) P73 (4, s5)	P22 (4, s3) P28 (2, s3) P67 (4, s5) P68 (4, s5) P70 (1, s5) P80 (1, s5) P84 (2, s2)	**	P11 (4, s3) P15 (5, s3) P16 (1, s3) P17 (5, s3) P22 (2, s3) P24 (4, s3) P28 (4, s3) P46 (5, s3) P47 (5, s3) P49 (4, s3) P70 (1, s4) P74 (4, s5) P82 (4, s5) P83 (1, s4)
2. operating cost		**	P4 (4, s4) P5 (1, s3) P6 (4, s3) P8 (4, s3) P9 (2, s3) P20 (2, s3) P23 (1, s3) P46 (5, s3) P52 (5, s3) P57 (2, s4) P59 (2, s4) P60 (4, s3) P61 (4, s3) P63 (3, s2) P64 (3, s3) P76 (3, s5)	P4 (4, s4) P6 (4, s3) P8 (4, s3) P9 (2, s3) P21 (1,s3) P28 (3, s3) P48 (1, s3) P50 (2, s3) P54 (1, s5) P58 (1, s4) P65 (3, s3) P66 (1, s4) P75 (1, s5) P78 (1, s5) P81 (1, s5) P85 (1, s3) P86 (1, s2)	P8 (4, s3) P13 (3, s3) P18 (3, s3) P33 (3, s3) P41 (3, s3) P42 (4, s3) P59 (4, s4) P61 (4, s3)	P22 (1, s3) P23 (1, s3) P39 (4, s3) P43 (1, s3) P48 (1, s3) P53 (1, s3) P62 (1, s3) P67 (1, s5) P68 (1, s5) P70 (4, s5) P81 (4, s5) P84 (3, s2) P86 (2, s2)	**	P14 (3, s3) P15 (5, s3) P16 (1, s3) P17 (5, s3) P19 (1, s3) P22 (4, s3) P27 (4, s3) P39 (4, s3) P41 (3, s3) P42 (4, s3) P43 (1, s3) P48 (3, s3) P50 (4, s4) P52 (1, s4) P64 (1, s3)
3. product quality & amount			**	P1 (1, s3) P3 (1, s1) P4 (1, s4) P6 (4, s3) P9 (4, s3) P55 (4, s4) P72 (4, s5) P79 (1, s5)	P33 (3, s4) P59 (1, s3) P61 (1, s3) P73 (1, s5) P75 (3, s5)	P23 (1, s3) P40 (1, s3) P53 (1, s3) P57 (1, s3) P59 (3, s4) P79 (1, s4) P84 (3, s3)	P31 (1, s3) P32 (1, s3) P33 (1, s3) P34 (1, s3) P35 (1, s3) P36 (1, s3) P37 (1, s3) P38 (1, s3)	P12 (3, s3) P20 (1, s3) P24 (3, s3) P32 (1, s3) P33 (1, s3) P34 (1, s3) P35 (1, s3) P36 (1, s3) P37 (1, s3) P38 (1, s3) P46 (5, s3) P49 (1, s3) P51 (1, s3) P57 (1, s3) P64 (4, S3) P74 (1, s5) P79 (1, s5)
4. environmental impact				**	P8 (3, s3)	P28 (2, s4) P59 (5, s3) P81 (4, s5)	**	P48 (3, s3) P50 (4, s3) P79 (1, s5)
5. safety					**		**	P13 (1, s3) P18 (3, s2) P33 (4, s3) P41 (2, s3)

								P42 (1, s3) P75 (3, s5)
6. complexity						**	P31 (1, s3)	P20 (1, s3) P22 (1, s3) P25 (1, s3) P26 (1, s3) P27 (4, s3) P28 (4, s3) P29 (1, s3) P30 (1, s3) P31 (1, s3) P39 (1, s3) P40 (1, s3) P42 (1, s3) P43 (1, s3) P57 (1, s3) P69 (1, s4) P70 (1, s4) P79 (2, s4) P84 (1, s3)
7. flexibility							**	P31 (1, s3) P32 (1, s3) P33 (1, s3) P34 (1, s3) P35 (1, s3) P36 (1, s3) P37 (1, s3) P38 (1, s3)
8. controllability								**

Table 2. Heuristics for reactor/separator system

Heuristics	**Key parameters**	**Objective issues**
P1 - minimizing the reactor volume/ maximizing reaction selectivity based on the most appropriate concentration profile.	reaction rate reaction selectivity	capital cost, product quality
P2- using an excess of one of the reactants	reaction rate raw material efficiency	capital cost, operating cost
P3- feeding inert material to the reactor or separating the product partway before carrying out further reaction.	product specification	capital cost, product quality
P4- recycling unwanted by-product to reactors	reaction rate reaction selectivity	capital cost, operating cost, environmental impact
P5- recycling of unconverted reactant to reactors.	raw material efficiency	operating cost, product quality
P6- treating the by-product as a product, as fuel, or via extensive waste-treatment process.	by-product recovery efficiency	capital cost, product quality
P7- purifying the impurities before reactions to avoid the additional by-products	reaction selectivity product specification	capital cost, product quality
P8 - increasing reaction rate to avoid producing components of highly corrosive nature, or which might polymerise or decompose to undesirable by-products.	reaction rate product specification	product quality, operating cost, environmental impact, safety
P9 - increasing the conversion of complex reactions result in the formulation of by-products and the decrease of the product impurities.	reaction conversion product specification	product quality, environmental impact
P10 - optimising the optimum conversion which involves a trade-off between large reactor cost at high conversion and large recycle costs at low conversions.	reaction conversion recycle ratio	capital cost, operating cost
P11 - optimising the optimum conversion which involves a trade-off between reactor costs and the raw material cost.	reaction conversion raw material efficiency	capital cost, operating cost
P12 - applying different reactors when reactions take place at very different temperatures or pressures, or if different catalysts are used.	reaction rate reaction conversion	capital cost, product quality, controllability,
P13 - optimising the reactor temperature by safety considerations, materials of construction limitations, maximum operating temperature for the catalyst,	reaction rate reaction conversion	safety, controllability
P14 - increasing the pressure of irreversible V-phase reactions will increase the rate of reaction.	reaction rate	operating cost, controllability
P15 - optimising the reaction pressure for V-phase reversible reactions depend on whether there is a decrease or increase in the number of moles and whether there is a system of single or multiple reactions.	reaction rate	product quality, safety, controllability
P16 - operating the reaction in liquid phase is preferred for maintaining the high concentration. There is more rapid reaction and it leads to smaller reactor volume;	reaction rate	capital cost, operating cost, controllability,
P17- deciding the reacting phase by trading off mass transferring rate and reaction kinetics to minimize the reactor volume for multiphase system	reaction rate	capital cost, operating cost, controllability
P18 - operating the reaction in gas phase for safety consideration, such as the critical temp of chemical species, or extremely high pressure maybe required to operate in liquid phase, so then reactor must be in gas phase.	reaction rate product specification	safety, controllability
P19 - improving the reaction rate by selecting the catalyst	reaction rate	operating cost, controllability
P20 - selecting the heterogeneous catalyst rather than homogeneous ones.	reaction rate reaction selectivity	product quality, complexity, controllability
P21- separating and recycling of the homogeneous catalyst	raw material efficiency	capital cost, operating cost, environmental impact
P22 - deciding the heat transferring operation from easy to difficult, from adiabatic operation to indirect heat transfer, then offering high temperature and heat flux.	energy consumption efficiency	operating cost, complexity, controllability,

P23 - cooling the reaction product by direct contact with a cold fluid. Use of extraneous materials should be avoided.	product specification	product quality, operating cost, complexity
P24 - dividing the reactor up into adiabatic bed and using interchangers for the reversible and exothermic reactions for adjusting temperature changes.	energy consumption efficiency	capital cost, controllability
P25 - dividing the separation systems into vapour recovery system and a liquid separation system.	separation efficiency	complexity, controllability
P26 - deciding the type of the separation system via the state of the reactor outlet flow a. If the reactor effluent stream is a liquid, use liquid separation system. b. If the reactor effluent is a two-phase mixture, phase-split the stream and sent them to liquid and vapour recovery system. c. If the reactor effluent is all vapour, then cool the stream to cooling water temperature and attempt phase split. Send the flash liquid and flash vapour to liquid and vapour recovery system.	separation efficiency	complexity, controllability
P27 - separating the homogeneous mixture by adding another phase, such as a solvent	separation efficiency	operating cost, complexity, controllability
P28 - using the solvent for separating rather than phase separation	separation efficiency	capital cost, complexity, controllability
P29 - separating the heterogeneous or multiphase mixture by exploiting differences in density between the phases.	separation efficiency	complexity, controllability
P30 - separating the different phases of a heterogeneous mixture should be carried out before homogenous separation.	separation efficiency	complexity, controllability
P31 - selecting the easy separating technique, such as distillation, under the separation requirement	separation efficiency	complexity, flexibility, controllability
P32 - selecting the absorption, adsorption and membrane gas separation for the low molecular weight material, instead of the distillation.	separation efficiency	product quality, controllability
P33 - using vacuum or reduced distillation for the high-molecular-weight heat sensitive materials	separation efficiency	safety, controllability,
P34 - using the adsorption and absorption for separating the components with a low concentration instead of distillation.	separation efficiency	product quality, flexibility, controllability
P35 - using other techniques for separating the classes of components instead of distillation	separation efficiency	product quality, flexibility, controllability
P36 - using extractive or azeotropic distillation for low relative volatility or exhibiting azeotropic behaviour. Crystallization and liquid-liquid extraction also can be used	separation efficiency	product quality, flexibility, controllability
P37 - using evaporation and drying for separating a volatile liquid from an involatile component.	separation efficiency	product quality, flexibility, controllability
P38 - using partial condensation followed by a simple phase separator give a good separation for separation of mixture of condensable and non-condensable components.	separation efficiency	product quality, flexibility, controllability
P39 - separating the components by their normal boiling point. If $\alpha < 1.1$, find a distillation sequence to separate the revise list of components	separation efficiency	complexity, controllability
P40 - sequencing columns by those heuristics for the recovery of the lightest component first; the recovery of the most plentiful component first; making the most difficult splits last; favouring equivocal splits	separation efficiency	product quality, complexity, controllability

P41 - selecting the higher pressure of distillation for less operating cost	separation efficiency	operating cost, safety, controllability,
P42 - selecting the lower pressure of distillation for easy controllability and safety considerations.	separation efficiency	operating cost, safety, controllability,
P43 - selecting the distillation pressure to allow a pressure above ambient, to allow cooling water or air cooling to be used in the condenser	separation efficiency	operating cost, complexity controllability,
P44 - selecting the reflux ratio based on the capital energy trade-off for the stand-alone distillation column.	separation efficiency	capital cost, operating cost
P45 - selecting the optimal reflux ratio of the heat-integrated column is different from that for a stand-alone column since the nature of the tradeoffs changes.	separation efficiency	capital cost, operating cost
P46 - deciding the feed condition by trading off the cost and product quality	separation efficiency	capital cost, operating cost, product quality
P47 - deciding the operating parameters for the distillation system based on the heat-integration strategies.	separation efficiency energy consumption efficiency	capital cost, operating cost
P48- using the pressure change alters the azeotropic composition before use of an extraneous mass separating agent.	separation efficiency	operating cost, environmental impact, controllability
P49 - using two columns operated at different pressure for separating azeotrope if the composition of the azeotrope is sensitive to pressure and if it is possible to operate the distillation over a range of pressures.	separation efficiency	capital cost, product quality, controllability
P50 - using an extraneous material for azeotropic distillation if the azeotrope is not sensitive to changes in pressure.	separation efficiency	operating cost, environmental impact, controllability
P51 - selecting the solvent for the azeotropic distillation based on its chemical structure similar to that of the less volatile of the two components.	separation efficiency	product quality, controllability
P52 - deciding the flow rate of solvent to achieve a better separation	separation efficiency	product quality, operating cost,
P53 - selecting the entrainer or solvent that already exist in the process.	separation efficiency product specification	operating cost, product quality, complexity
P54 - separating and recycling the unreacted feed via pump (liquid) and compressor (vapour).	separation efficiency recycle ratio	capital cost, operating cost, environmental impact
P55 - dealing with the by-product via separating and removing	separation efficiency	capital cost, product quality
P56 - dealing with by-product via purge.	emission ratio	capital cost, environmental impact
P57 - sequencing the separation columns based on the order of volatility between the separated components among product, by-product and feed.	separation efficiency	product quality, complexity, controllability
P58 - recycling the by-products for reversible reaction.	recycling ratio reaction conversion	capital cost, operating cost, environmental impact,
P59- removing the components which are damaged for catalyst before recycling.	separation efficiency	capital cost, product quality, safety
P60 - removing the large amount of purities which can be separated easily by distillation before processing the feed stream.	separation efficiency	capital cost, operating cost, product quality
P61 - separating the impurities which have an adverse effect on the reaction or poison the catalyst before they enter into reactor	separation efficiency	operating cost, product quality, safety
P62 - feeding the impurity produced into the process at the point where the impurities are removed or recovered	separation efficiency	operating cost, complexity
P63 - processing the impurities along the reactor when impurities do not have a significant effect on the reaction.	reaction conversion	capital cost, operating cost, product quality
P64 - processing the impurities which are in the gas phase	reaction rate	operating cost, product quality, controllability

P65 - purging the impurities when there is no harm and expensive separation between feed and impurities	emission ratio	operating cost, environmental impact
P66 - recycling the diluents and solvents if they are needed in the reactor.	recycling ratio	capital cost, operating cost, environmental impact
P67 - reusing the extraneous amount of the heat carrier. It may affect the recycle structure of the flowsheet.	recycling ratio	capital cost, operating cost, complexity
P68 - recycling the material of the process as the heat carrier instead of introducing extraneous materials into the process.	recycling ratio energy consumption efficiency	capital cost, operating cost, complexity
P69 - recycling structure of the heat carrier based on the volatilities of the components (product, feed, other heat carrier)	recycling ratio	complexity, controllability
P70 - avoiding unnecessary separation and unnecessary mixing	product yield	capital cost, complexity controllability,
P71 - using gas recycle and purge if a feed impurity or a reaction by-product boil at a lower temperature than propylene	recycling ratio emission ratio	capital cost, environmental impact controllability,
P72 - purging the gas impurity in gas reactant instead of recovering it	emission ratio	capital cost, environmental impact
P73 - using vapour recovery system on the gas recycle stream if the flash vapour stream contains components that foul the catalyst	separation efficiency	capital cost product quality, safety
P74 - using the vapour recovery system on the gas recycle stream if the flash vapour stream contains components that upset the reactor operability.	separation efficiency	capital cost, product quality controllability,
P75 - using the vapour recovery system on the purge stream if it contains a large amount of valuable components	separation efficiency	operating cost, capital cost, environmental impact
P76 - removing the light ends if they contaminate a product stream.	separation efficiency	product quality, capital cost
P77 - dealing with the light ends as a fuel supply if no significant amount of valuable materials leave with the light ends stream.	by-product recovery efficiency	capital cost, environmental impact
P78 - recycling the valuable material from the light end	recycling ratio	capital cost, operating cost, environmental impact
P79 - using partial condensation followed by a simple phase split when the reactor effluent contains components with a wide range of volatilities.	separation efficiency	product quality, environmental impact, controllability
P80 - removing the vapour stream of the phase split if it is either predominantly product or predominantly by-product.	separation efficiency	capital cost, environmental impact, complexity,
P81 - recycling the vapour stream to the reactor if it contains predominantly unconverted feed materials	recycling ratio	capital cost, operating cost, environmental impact
P82 - using the expensive recycle compressor for the vapour recycles if it needs very high pressure or very low levels of refrigeration.	recycling ratio	capital cost, controllability
P83 - using liquid recycle instead of vapour recycle by avoiding the compressor	separation efficiency	capital cost, controllability
P84 - using further reaction to upgrade the product value.	product yield raw material efficiency	capital cost, operating cost, complexity
P85 - purifying the feed to avoid the loss of useful material in the purge streams	product yield separation efficiency	capital cost, operating cost, environmental impact
P86 - using additional reactor on the purge streams avoiding the loss of useful material	product yield raw material efficiency	capital cost, operating cost, environmental impact

Table 3. Guidewords for the heuristic study

Indicators		Explanation
I_1 =1	The more, the more	applying the heuristic will improve the objective in the cell of left column, also improve the objective in cell of the top row
I_2 =2	The less, the less	applying the heuristic will decrease the objective in the cell of left column, also decrease the objective in the cell of the top row
I_3 =3	The more, the less	applying the heuristic will improve the objective in the cell of left column, however decrease the objective in the cell of the top row
I_4 =4	The less, the more	applying the heuristic will decrease the objective in the cell of left column, but improve the objective in the cell of the top row
I_5 =5	uncertain	the function of applying the heuristic is uncertain
S1	feed /input	applying the heuristic to the region of feed/input in the flowsheet structure
S2	reaction	applying the heuristic to the region of reaction in the flowsheet structure
S3	separation	applying the heuristic to the region of separation in the flowsheet structure
S4	recycle	applying the heuristic to the region of recycle in the flowsheet structure
S5	output	applying the heuristic to the region of output in the flowsheet structure

Table 4. The list of Process Parameters for the heuristic study

Objective	Process Property Parameter	Process Operating Parameter
ob1. capital cost	ph1. raw material efficiency	p1. feed component constraints
ob2. operating cost	ph 2. reaction rate	p2. feed flow rate
ob3. product quality/amount	ph 3. reactor conversion	p3. feed flow temp
ob4. environmental impact	ph 4. reaction selectivity	P4. feed flow pressure
ob5. safety	ph 5. separation efficiency	p5.reactant concentration
ob6. complexity	ph 6. recycling flow rate/ratio	p6. reaction kinetics
ob7. flexibility	ph 7. emission ratio	p7. reaction catalyst
ob8. controllability	ph 8. product specification	p8. reaction phase
	ph 9. product yield	p9. reaction temp
	ph 10. by-product recovery efficiency	p10. reaction pressure
	ph 11. energy consumption efficiency	p11. reaction resident time
		p12. separating component
		p13. separation sequence
		p14. separation agent
		p15. No. of columns
		p16. separation temp
		p17. separation pressure
		p18. Number of recycling flows
		p19. Number of compressors
		p20. Number of purging flows

APPENDIX II Distillation System Conflict Table

Table 1. Conflict table of process characteristics for distillation system

CHARACTERISTICS		Characteristics that are getting worse										
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
1	feed conditions	***	2, 7, 8, 6, 1, 3, 13	2, 1, 3	-*	2, 3, 1, 6, 7, 8	6, 8	6, 7	12, 11, 10, 6	6, 7, 14	6, 8, 7	6,7, 14, 4
2	separation specification	6, 12	***	-	1, 3	-	8, 1, 3	7, 1, 6, 15	11, 10, 12, 2, 5	6, 1	6, 1	2, 6, 7, 14
3	constraints of comp.	1, 2, 3	2, 1, 3	***	1, 3, 2	2, 1, 6	6, 8	7, 2, 1, 3, 6	12, 10, 11, 3	6, 2, 14	6, 2, 1	6, 4
4	separation agent	-	1, 2	2, 1, 6	***	2, 1, 6	8, 7	7, 6, 9, 15	12, 10, 11, 5	6, 14	6, 14	6, 4, 14
5	relative volatilities	6	2, 7, 8	-	2, 1, 3	***	8	6, 2, 9, 15	11, 10, 12, 5	6, 14	6, 8	2, 4, 6
6	reflux ratios	-	8, 2, 1, 6	-	1, 2, 6	-	***	8, 6	12, 11	8, 6	-	4, 6, 16, 20
7	number of trays	-	7, 6	-	3, 1, 2	-	7, 12	***	7, 11, 10	-	-	-
8	purge conditions	-	12, 10, 1, 2, 6	-	1, 2, 3	-	8, 6, 7	7, 12, 11	***	6, 14		-
9	temperatures	6	7, 8, 11, 10	2, 3, 15, 9	1, 2, 3	2, 3, 1	-	-	12, 7, 8, 11	***	6, 8	4, 14
10	Pressures	6	7, 8	2, 1, 6, 15, 9	2, 1, 3	7, 8, 2, 1	8, 12	7, 20, 15, 9	11, 10	21	***	14, 4
11	energy flow	-	-	11, 2	-	7, 8	8, 6	7, 6	12, 11, 10	21, 6	21	***
12	mass flow	-	3, 1, 5	2, 3, 1, 11	3, 2, 1	3, 1, 7	8, 6	7, 6	12, 5, 11, 10	-	21, 6	6, 14
13	number of columns	-	9, 1, 2, 3, 7	6, 2, 3, 1	2, 1, 9	6, 3, 2, 1	8, 9	7, 1, 2, 3	11, 10, 12, 5	14, 6, 2, 3	14, 6, 2	6, 14, 4
14	condenser number	-	6, 7, 8	11, 10, 12	-	-	8, 6	7, 20	11, 10	14, 6	14, 6	6, 14
15	reboiler number	-	6, 7, 8	10, 11, 12	-	-	6, 8	7, 20	10, 11	14, 6	14, 6	6, 14
16	heat exchanger number	-	6, 11, 10	-	-	-	-	-	6, 10, 11	6, 14, 11, 10	6, 14, 11, 10	4, 6, 14
17	compressor number	-	-	6, 11, 10	-	6, 8	7	6	10, 11	6	6	18, 16, 17, 19
18	hot utility levels	6	6, 7, 8	6, 2, 3	1, 2, 6	-	-	-	11, 10, 12	6, 4, 16~20	6, 4, 16~20	4, 15 16~20
19	cold utility levels	6	6, 7, 8	6, 2, 1	1, 2, 3, 6	-	-	-	11, 10, 12	6, 4, 16~20	6, 4, 16~20	4, 15 16~20
20	number of recycles	-	11, 12, 10, 5	12, 11, 10	1, 2, 3	-	12, 11, 8	7, 6	12, 11, 5	6, 11, 4	6, 11, 4	11, 4
21	number of purges	-	2, 12, 11, 10, 5	12, 11, 10, 2	2, 1, 3	-	8, 11, 10	7, 11, 10	12, 11, 10, 5	-	-	-
22	uncertainties	-	6, 7, 8, 10, 11	2, 3, 1	1, 2	29, 26	29, 27, 28	6, 7, 28, 29	12, 11, 10, 5	29, 26, 27	29, 26, 27	29, 26, 27, 6
23	complexity	-	1, 3, 21, 25	21, 25, 27	1, 3	-	-	-	5, 11, 10	3, 2, 1, 6	1,3, 2, 6	25, 5, 16~20

(continued)

CHARACTERISTICS		Characteristics that are getting worse										
		12	13	14	15	16	17	18	19	20	21	22
1	feed conditions	12, 2, 11, 5	8, 9, 15, 1, 3, 2	20, 19, 15, 17	20, 19, 16, 17, 15	4, 16	6, 10, 11, 12	14, 6, 16, 20	14, 6, 16, 20	12, 11, 2	10, 11, 12	23, 27, 28, 25
2	separation specification	12, 11, 5	2, 9, 15, 8	20, 19, 17, 11	20, 16, 17, 15	4, 11, 6, 16	6, 10, 11	6, 14, 20, 16	6, 14, 20, 16	11, 10	5, 10, 11	23, 27, 25, 28
3	constraints of comp.	12, 11, 5	9, 2, 15, 8	20, 19, 17, 4	20, 19, 17, 4	4, 11	11, 6, 4	6, 20, 16	14, 20, 6	11, 10, 2	12, 10, 11, 5	21, 24, 25
4	separation agent	12, 11, 5	2, 8, 9, 15	-	-	-	-	6, 20, 16	20, 6	12, 11, 10, 2	12, 11, 5, 10	21, 23, 24, 25
5	relative volatilities	5, 3, 2, 6	2, 8, 15, 13	20, 19, 17, 4	4, 16, 19, 20	4, 17, 11	10, 11, 4	6, 20, 16, 19	6, 16, 20	11, 12, 2	12, 10, 11	21, 24, 28
6	reflux ratios	8, 12	-	-	-	-	-	-	-	-	12, 11	8, 21
7	number of trays	-	9, 20, 15	20, 15, 19, 17	20, 19, 15, 16	-	-	-	-	-	-	7
8	purge conditions	12, 3, 1, 5	8, 15, 9	6, 12, 11, 10	-	-	-	-	-	12, 11, 6	12, 11, 10, 5	21, 22, 25
9	temperatures	3, 12, 5	9, 15, 20	20, 19, 17, 15	20, 19, 16, 17	4, 16	4, 11, 10	14, 4, 16~20	14, 4, 16~20	12, 11	12, 11, 10, 5	21, 29
10	Pressures	3, 2, 1	9, 15, 20	20, 19, 17, 15	20, 19, 16, 17	4, 16	4, 10, 11	14, 4, 16~20	14, 4, 16~20	11	10, 11, 5, 12	21, 27, 25
11	energy flow	3, 2, 1	20, 15, 19, 9	20, 19, 17, 16	16, 20, 19, 17	4, 16, 11	11, 10, 4	6, 7, 14	6, 7, 14	4, 11	4, 5, 11, 10	26, 27
12	mass flow	***	2, 3, 9, 15	-	-	-	-	-	-	12, 11, 5, 4	10, 11, 12, 5	26, 27, 21
13	number of columns	3, 2, 1	***	20, 19, 15, 17	20, 19, 16, 17	6, 4	11, 10, 18	6, 2, 3	6, 2, 3	11, 12, 9	5, 10, 10	21, 27, 25, 26
14	condenser number	-	20, 19, 9, 15	***	16, 17, 9, 20	4	18, 10, 11, 6	6, 14, 16~20	6, 14, 16~20	11, 2	11, 10, 5	26, 6, 7, 28
15	reboiler number	-	20, 19, 15, 9	17, 18, 20, 19	***	4	18, 6	6, 14, 16~20	6, 14, 16~20	11, 2	12, 10, 11, 5	26, 27
16	heat exchanger number	-	-	20, 19, 17, 16	20, 17, 19, 16	***	18, 6	6, 14, 16~20	6, 14, 16~20	11, 10	10, 11, 12	26, 21, 27
17	compressor number	-	13, 8, 9	10, 11	-	6, 11, 4	***	6, 14	6, 14	6, 11	12, 10, 9	26, 21, 27
18	hot utility levels	-	-	20, 19, 17, 16	20, 16, 19, 17	4, 11	-	***	6, 14	-	-	26, 21, 25
19	cold utility levels	-	-	20, 19, 17, 16	20, 17, 16	4, 6, 11	-	6, 14	***	11, 10, 12	10, 11, 12	26, 21, 25
20	number of recycles	11, 5	-	12, 11	-	6, 4	6, 11, 2	-	-	***	12, 11, 5	25, 27, 26
21	number of purges	12, 5	-	10, 11	-	-	6, 10, 11	-	6, 14	11, 12, 2	***	21, 25, 26
22	uncertainties	26, 29	-	-	-	-	-	6, 14	6, 14	11	12, 11, 10	***
23	complexity	25, 5, 12	3, 1, 2, 9	4, 20, 19, 17	4, 20, 19, 17	4, 11, 6	6, 11, 4	-	-	3, 2, 11	6, 12	26, 25, 21, 27

(continued)

CHARACTERISTICS		Characteristics that are getting worse								
		23	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**
1	feed conditions	23, 22, 24, 25	7,1, 2, 9, 20, 15	4, 1, 2, 3, 16~20	10, 11, 12, 3, 5	23, 21, 24, 27	23, 22, 28, 25	22, 23, 25, 28	8, 13, 21	21, 25, 28, 27
2	separation specification	23, 22, 28, 24	9, 1, 2, 3, 7	7, 4, 1, 2, 16~20	3, 1, 5, 12, 11	27, 23, 21, 25	23, 24, 25	22, 23, 24, 28	7, 8, 13	25, 21, 28, 27
3	constraints of comp.	23, 24, 22, 28	2, 1, 8, 7	2, 1, 3, 4	5, 3, 12, 11	23, 21, 27, 25	22, 24, 23	23, 22, 24	13, 8	21, 25, 28, 27
4	separation agent	23, 24, 28	2, 7, 8, 15, 13	2, 4, 9	10, 5, 12, 11	21, 24, 23	2, 1, 23, 24	2, 1, 22, 24	13, 8, 7	21, 28
5	relative volatilities	23, 24, 22, 25	8, 9, 15	2, 7, 1	5, 11, 10, 12	24, 23, 27	2, 23, 24, 22	23, 22, 24, 28	1, 2, 8	-
6	reflux ratios	23, 24	7, 13, 15	4, 16~20	12, 11, 10, 5	24, 23	22, 23, 24	22, 24, 23	8	-
7	number of trays	-	9, 15, 8, 13	7, 4	25, 21	21, 25	6, 7, 23	7, 6	21, 7	-
8	purge conditions	11, 22, 24, 25	9, 8, 13, 15, 20	9, 12, 4, 5	12, 10, 11, 5	12, 10, 21, 25	12, 6, 22, 24	11, 10, 22, 24	21, 9, 8, 13	21, 28
9	temperatures	22, 24, 23, 27	8, 9, 15, 20, 13	4, 7, 16~20	12, 11, 10, 5	21, 26, 25	12, 24, 22	22, 24, 28	7, 8, 9, 15	28, 21
10	Pressures	22, 23, 24, 28	8, 9, 13	4, 7, 16~20	10, 11, 12, 5	21, 27, 25	22, 24, 23	23, 22, 24, 28	7, 8, 9, 15	21, 28
11	energy flow	22, 23, 24, 28	9, 7	4, 16~20	4, 5, 12, 11	21, 25, 26, 27	29, 26, 22, 24	28, 22, 24, 26	21, 9	21, 27
12	mass flow	22, 24, 28	8, 9, 7	7, 5, 3, 1	5, 12, 11, 10	21, 25, 27	27, 29, 25	22, 23, 24, 28	21, 7, 8	21, 25, 27
13	number of columns	23, 22, 24	9, 7	3, 2, 1	11, 10, 12, 5	21, 27, 11, 10	26, 27	22, 24, 28	21, 2, 1	21, 28, 25
14	condenser number	21, 25	8, 9, 7	7, 3, 4, 16~20	12, 10, 11	21, 25	26, 29, 27	23, 22, 24, 28	9, 8	21, 28
15	reboiler number	21, 25	8, 9, 7	7, 4, 3, 16~20	12, 11, 10	21, 25	26, 29, 27	21, 22, 24, 28	9, 8	21, 28
16	heat exchanger number	22, 24	9, 20, 7	4, 16~20	11, 10, 12	21, 22, 25, 26	24, 22, 26	22, 24, 28, 25	6, 7	28, 21, 25
17	compressor number	23, 25	4, 6, 8, 17, 20	4, 7, 6, 16~20	12, 11, 10	23, 24, 21, 25	22, 24	22, 23, 24, 25	-	21, 28
18	hot utility levels	23, 27, 28	13, 8, 20, 19	4, 15, 16~20	3, 11, 12, 10	21, 25, 27	23, 26	22, 23, 24, 28	21	28, 21
19	cold utility levels	23, 27, 28	13, 8, 20, 17	4, 15, 16~20	3, 11, 12 10	21, 25, 27	23, 26, 24	22, 23, 24, 28	21	21, 28
20	number of recycles	22, 23	13, 15, 9	9, 7, 4	12, 11, 10, 5	21, 22	22, 23, 26	22, 24, 23, 28	21	25, 21, 28
21	number of purges	22, 24, 28	-	12, 11, 10, 6, 2	29, 26, 11, 10	21, 27, 25	22, 24, 26	22, 23, 24, 28	21, 25	28, 25, 21
22	uncertainties	29, 27, 26, 21	29, 26	26, 29, 27	12, 11, 25	21, 25	29, 27, 26	23, 27, 28, 25	21, 25	27, 26, 28, 21
23	complexity	***	9, 15, 13	1, 3, 2, 4	12, 11, 25	21, 25, 26, 27	22, 23, 24	23, 22, 24, 28	21, 13	28, 21

Table 2. Conflict table of objectives for distillation system

CHARACTERISTICS		Characteristics that are getting worse							
		24	**25**	**26**	**27**	**28**	**29**	**30**	**31**
24	capital cost	***	4, 7, 16~20	25, 26, 6	21, 27	25, 26, 6, 12	24, 23, 22	21, 9	28, 21, 25
25	operating cost	9, 4, 15, 7	***	25, 21, 26, 27	21, 27, 25	22, 24, 23, 25	23, 22, 24, 28	21, 13, 9	28, 25
26	environmental	9, 15, 13	1, 3, 2, 9, 5	***	21, 25, 27	23, 22, 24, 26	22, 24, 23, 28	21, 25, 9	21, 25, 28
27	safety	9, 2,1	1, 3, 2, 4	3, 1, 2, 5	***	22, 23, 24	22, 24, 23, 28	21, 25	27, 26, 28, 21
28	flexibility	9, 7, 6, 23	8, 9, 4, 13	12, 11, 10	21, 25, 26, 27	***	23, 22, 24, 28	25, 21	25, 28, 27
29	controllability	9, 6, 7	8, 4, 9	21, 25, 12, 11	25, 21, 5, 3	23, 22, 24, 25	***	21, 25	28, 25, 26
30	capacity	9, 4, 7, 13	1, 4, 8, 8, 8, 13	21, 12, 5, 10	21, 25, 27, 26	22, 24, 23, 26	23, 22, 24, 28	***	21, 25, 28
31	life cycle	9, 4, 1, 2	1, 4, 9, 2, 3	3, 12, 11, 10	21, 27, 26	23, 24, 22, 26	22, 23, 24, 28	21, 28	***

Table 3. Conflict table of objectives to process characteristics for distillation system

CHARACTERISTICS		Characteristics that are getting worse							
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
24	capital cost	-	9, 15, 20	21, 25	1, 2, 3	3, 6	8	7, 6	10, 11, 12
25	operating cost	-	1, 3, 2	2, 6, 21	1, 3, 2, 4	1, 3, 2	8	7, 9	5, 11, 10, 3
26	environmental	-	12, 2, 3, 1	6, 3, 2, 1	1, 3, 5	3, 1	8	7	12, 11, 10, 5
27	safety	-	21, 26, 27	27, 25, 21	1, 3	3, 1	8, 6	7, 6	12, 11, 10, 2, 5
28	flexibility	6, 7, 8, 12	7, 8, 6, 13	6, 7, 8, 2, 5	1, 2, 3	-	8, 6	6, 7	11, 10, 12, 6
29	controllability	-	-	25, 26, 27	-	-	6, 8	6, 7	6, 12, 11, 10
30	capacity	-	21, 3, 1, 2, 9	2, 6, 9	1, 2, 3	3, 1	8, 6	9, 13, 6, 17	2, 11, 12, 10
31	life cycle	-	1, 3, 2	2, 3, 6, 11, 10	1, 2, 3	-	8	7	1, 2, 5, 10

(continued)

CHARACTERISTICS		Characteristics that are getting worse							
		9	**10**	**11**	**12**	**13**	**14**	**15**	**16**
24	capital cost	14, 11	14, 11	6, 14	-	9, 1, 3, 15, 20	20, 15, 19, 17	20, 15, 19, 17	4, 6, 11
25	operating cost	14, 6, 11, 4	14, 6, 11, 4	6, 4, 14	3, 5	9, 20, 15, 11	20, 17, 9	20, 17, 9	4, 11
26	environmental	2, 3, 6	6, 1	6, 4, 14	3, 5	9, 11, 10, 15	15, 9, 17, 20	15, 19, 17, 20	4, 6, 11, 10
27	safety	6, 1, 3	6, 1	6, 14	5, 12	9, 13	4, 15	4, 15	4, 11, 12
28	flexibility	14, 7, 8, 6	14, 6, 7, 8	6, 14	3, 7, 6	8, 9, 15	14, 6, 4	4, 14, 6, 17	4, 6, 11
29	controllability	21, 26, 14, 6	21, 26, 6	-	-	23, 9, 8	4, 15, 17	4, 15, 16, 17	6, 4, 11
30	capacity	3, 1, 2, 14, 6	1, 3, 6, 14	6, 7, 14	3, 1, 11, 10	9, 8, 6, 13	-	-	6, 11, 14
31	life cycle	1, 3, 6, 14	1, 3, 6	6, 7	3, 1, 10, 11	9, 8, 1, 3, 2	6, 4	6, 4	4, 6

(continued)

CHARACTERISTICS		Characteristics that are getting worse							
		17	**18**	**19**	**20**	**21**	**22**	**23**	
24	capital cost	6, 11, 10	-	-	12, 11	12, 11, 10, 5	29, 26	24, 23, 27	
25	operating cost	6, 11, 10	6, 4, 16~20	6, 4, 16~20	11, 20, 23, 24	11, 10, 23, 12	25, 21, 26	23, 22, 24, 28	
26	environmental	-	6, 4, 11, 10	6, 4, 14, 11	12, 11, 5	12, 10, 11, 5	21, 25, 26, 27	21, 22, 24, 27	
27	safety	-	6, 14	6, 14	22, 23, 24, 11	12, 11, 10, 24	25, 21, 26, 27	22, 23, 24, 25	
28	flexibility	6, 11	6, 11, 14	6, 14, 11	22, 24, 11, 10	5, 11, 12, 10	21, 26, 27, 28	22, 24, 23, 25	
29	controllability	6, 11, 10	-	-	11, 22, 24, 23	12, 10, 11, 5	21, 25, 27, 26	23, 24, 22, 28	
30	capacity	6, 10, 11, 12	6, 14	6, 14	12, 11, 9	12, 10, 11	21, 27, 26, 25	23, 22, 24, 28	
31	life cycle	6, 11, 10, 2	6, 14	14, 6	12, 9, 11, 2	2, 3, 12, 10	25, 21, 27, 26	23, 22, 24, 28	

‘-’ means no relevance.

APPENDIX III Waste Minimization Conflict Table

Table 1. Conflict table for waste minimization

Characteristic of WM	**Design Objectives**							
	E1	E2	E3	E4	E5	Q1	Q2	Q3
1	H1, H5, H6(+), H11(-)	H1, H4(-), H5, H30(-)	-	H1	-	H1	-	H3, H4(+), H5(+), H11(+), H30(+)
2	H1, H2(+), H3, H11(+), H12(+), H22(+), H24(+)	H11(+), H30(-)	-	H3	H11(-), H30(-)	-	H2(+), H22(+)	H3, H22(+), H24(+), H30(+), H31
3	H12(+)	H5, H6(+), H13	-	H3, H12(+)	-	H5, H14(+), H22(+)	H12(+)	H3, H11(+), H14(+)
4	-	H4(-), H5, H6(+), H13	-	H13	-	H5, H14(+)	-	H3, H4, H13, H14(+)
5	H15	-	-	-	-	H15	-	H15(+)
6	-	H16, H17(+)	-	-	-	-	-	H15(+), H16(+), H17(+), H29(+)
7	H22(+), H23(+), H24(+),	H22(-), H24(+)	-	-	-	-	-	-
8	-	H21(-), H(28)	-	-	-	-	-	-
9	-	H25(+)	-	H25	-	-	-	-
10	-	H28	-	H25, H28	H9(+)	H1	H2, H31	H3, H26, H28, H31
11	-	H18, H19(+), H20(+)	H18(+), H19(+), H20(+)	-	-	-	-	-
12	H22(+)	H7, H8, H13, H16, H17, H18, H19(+), H20(+), H22(-), H23, H24, H28, H30(-)	H18(+), H19(+), H20(+)	H28	-	-	-	H16, H17, H28, H30(+)

(continued)

	S1	S2	S3	S4	C1	C2	C3	C4
1	-	-	-	-	H1, H4, H5, H6(-), H30	H5	-	H4(+), H30
2	-	-	H30(+)	-	H11(+), H30	H22, H24, H30, H31	H22(-), H24	-
3	-	H10(+)	-	H10(+)	H3, H5, H10, H12, H13, H14	H5, H6(+), H10, H14	-	H10, H14
4	-	-	-	-	H4(+), H5, H13, H14	H5, H6(+)	-	H4(+), H13, H14
5	-	-	-	-	H15	H15	-	
6	-	-	H29	-	H15, H16	H15, H16, H29	-	H16, H17
7	-	-	H22(+)	-	-	H22, H23, H24	H22, H23, H24	H24
8	-	H28	H21(+), H28	-	-	-	-	H21
9	-	-	H27(+)	-	-	H25, H27	-	-
10	-	-	H26(+), H27(+)	-	H1, H3, H9(+)	H9(+), H25, H26, H27, H31	-	H9(+)
11	-	-	-	-	H18, H19, H20	H18, H19, H20	-	H18, H19, H20
12	-	H7, H8	H22(+), H27, H30(+)	H7, H8	H7, H8, H13, H16, H17, H18, H19, H20, H30	H7, H8, H17(+), H18(+), H19, H20, H22, H23, H24, H27, H28, H30	H22, H23, H24	H7, H8, H13, H16, H17, H18, H20, H30

‘-’ means no relevance

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