AN INTEGRATED APPROACH TO THE DESIGN OF ENERGY EFFICIENT PROCESS SYSTEMS (IDEES)

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2. Executive Summary

"Integrated Approach to the Design of Energy Efficient Systems" – The phrase chosen as the title of this project reflects its integrated nature of approach to the problem of designing energy efficient and clean process systems. This approach has led to a co-ordinated activity encompassing four main areas:

1. A framework for process synthesis representation, site-wide considerations, life-cycle assessment and operational aspects in order to identify new processing routes leading to more energy efficient and clean processes.

2. A methodology, for solving the resulting mathematical models based on multi-objective optimisation and mixed integer programming techniques.

3. Development of computer-aided prototype tools that provide the platform for the effective implementation of the above representation framework, the methodology and the established techniques.

4. Industrial Applications, for testing and validating the developed tools, ensuring the technology transfer and improve current design and operational practice.

In the context of the research carried out in this project, a novel process synthesis representation has been developed and tested, based on fundamental physico-chemical phenomena (heat & mass transfer, chemical and phase equilibrium), which have enabled the conceptual identification of novel, hybrid processing routes and schemes requiring less energy and generate smaller amounts of waste. Energy requirements and waste generation have been assessed on a site-wide basis, i.e. by including the analysis of the energy generation plant and the processes providing the raw materials together with the conventional process system. The basis allows comparisons to be performed in a consistent and balanced way. Operational aspects, such as sequencing and scheduling, operability and safety, have also been explicitly incorporated into the analysis. The overall process synthesis/design model is represented by a novel multi-objective optimisation formulation, which has allowed the establishment of trade-offs amongst the design objectives of energy use, process economics and environmental impact. Decomposition algorithms employing mixed integer non-linear programming and global optimisation principles have been developed to efficiently solve the resulting large scale models. Parametric studies have also been performed to analyse the effect of variations in key parameters and process data on the design decisions. Two prototype computer-aided tools have been developed to support the entire design activity, encompassing all the process modelling techniques and representation methodologies as well as the corresponding numerical algorithms developed in the context of this project. The two tools have been tested and applied with success in the industrial case studies, achieving excellent potential for further development and exploitation.

The integrated design methodology developed in this project has established a formal link for (a) the representation of energy efficient separation systems, novel units and processes in a unified and consistent way and (b) their inclusion in a process engineering optimisation tool. In this context, it has achieved to complement and naturally extend other projects funded by the European Union. At the same time, it goes much beyond currently funded research in the Process Systems Engineering area, since it brings together elements of novel process synthesis and design representation, site-wide production routes and new optimisation techniques and tools for arriving at energy efficient, integrated and environmentally benign process systems.

3. Objectives of the Project

Over the last fifteen years substantial research effort has been devoted within the field of process systems engineering to heat/process integration as a framework for reducing energy requirements at the plant or even multi-site level. While indisputably significant industrial success has been recorded, yet, accumulated industrial evidence has started to show that innovative exploration of processing routes, schemes and process design options can, in fact, result in much higher reductions in energy consumption and costs compared to conventional processes. Such an example is the case of the Methyl Acetate process, where 50% reductions have been realised. Currently, however, almost all design methodologies and tools available in the Computer Integrated process engineering community are based on unit operations representations and as a result most heat integration studies so far have been limited to typical flowsheet patterns. Systematic techniques to reveal non-conventional innovative designs which require less energy and produce less waste, are clearly lacking. What is needed is a design methodology to help process engineers identify new processing routes which are more energy efficient, clean and economical.

Such a methodology requires a process representation based on physico-chemical phenomena, fundamental understanding of phase equilibrium and mass/heat transfer mechanisms in conjunction to process design alternatives, and means and techniques for representing, co-ordinating and optimising the simultaneous considerations of energy, process economics and pollution prevention. Addressing all these challenges, which is the scope of this project, requires a high degree of innovation. The research and development activity of the consortium has ensured that the project outcome is innovative in:

- advancing the current state of the art regarding the representation of process synthesis and design alternatives in order to identify new, more energy efficient and integrated production schemes, causing less environmental damage.

- establishing new integrated design methodologies for the solution of this type of problems.

- developing and applying advanced techniques for the rigorous optimisation of the integrated design model, to minimise energy usage, environmental pollution and costs.

More specifically, the industrial objectives of this project can be summarised as follows:

1. Development of a novel process synthesis framework based on fundamental physico-chemical phenomena (heat and mass transfer, chemical and phase equilibrium), which will enable the conceptual identification of novel (and

possibly hybrid) processing routes and schemes requiring less energy and smaller amounts of waste.
2. Validation and refinement of the proposed mathematical model for the synthesis of energy efficient process systems, based on a mass/heat transfer modular representation framework.
3. Assessment of energy requirements and waste generation on a site-wide basis, i.e. including the energy generation plant and the processes providing the raw materials, together with the conventional process system, in the analysis.
4. Investigation of multi-objective optimisation techniques for the solution of multi-objective synthesis problems, involving discrete and continuous decisions.
5. Investigation of a prototype software tool to support the entire design activity.

The Case Studies provided by the industrial partners STATOIL, WISAPAK have been carried out in order to test and further refine the proposed integrated process synthesis framework. A first sub-task focusing on refinery/petrochemical plant, concentrates on the verification of the synthesis representation part and its corresponding methodology. A second sub-task, dealing with a paper mill, mainly focuses on the site wide and operational aspects in conjunction with the developed numerical techniques. A third sub-task focuses on the synthesis aspects with respect to flowsheet, energy integration and operability issues. All three sub-tasks involve complex processes with high energy requirements.

Novel synthesis representations and generic methodologies and tools will lead to new process design routes consuming 'at source' less energy and emitting less wastes which should be translated not only to better design and operation of existing processes, but also to the development of new ones with more desired features. Europe has a good track record in the development of process systems engineering as a discipline of its own. The work undertaken in this project will ensure that this position is maintained and strengthened through the development of even more generally applicable tools for integrated design.

It is expected that developments of new technology and systematic methods for designing it, so as to achieve energy reductions and environmental benefits, will improve the competitive position of the EC processing industries. Such an integrated design methodology will not only develop improved processes, it will develop them faster: many of the labour-intensive, trial-and-error parts of the design processes will be automated. Thus, EC process industry will get new products and processes to market quicker, further improving their competitive position. Substantial consequential benefits will be also achieved by (a) the European chemical process and equipment design and manufacturing companies, (b) many small EC companies that supply them with special components, and (c) EC software development firms that supply specialised software services to the process industry.

The two operating companies in the consortium STATOIL, WISAPAK have immediate applications (refinery or petrochemical and paper mill) for which the tools developed within the project can be used. They therefore intend to do so as soon as these tools become available. Clearly, such use will continue beyond the end of the project.

The software company QUANTISCI, the research institutions ICEHT, CPERI and the universities IMPCOL, AAU, DTU involved are also committed to exploiting the new market opportunities opened by the additional capabilities (in modelling and optimisation tools for integrated design activities), both individually and jointly, where appropriate through an active marketing strategy of the integrated design tools resulting from this project to other companies in Europe, which can benefit from the results of this project. Imperial College IMPCOL and Technical University of Denmark DTU have industrial consortia (involving many of the leading European companies) and intend to use European events organised every years as an opportunity to bring the results of the project to the attention of the wider process engineering community. The software tools will be supplied to universities and other educational non-profit organisations at preferential prices.

4. Scientific and Technical Description of the Project

4.1 Task [T1]: Development of a Unified Framework

There are several issues that are to be addressed in the course of this task. In brief what is set to be accomplished is a process synthesis prototype tool that:

- explores alternative reaction schemes and intermediate process materials
- selects the most appropriate reactor configurations and separation sequences
- expands the process system boundaries beyond the on-site battery limits in terms of the energy generation and the process providing the raw materials
- introduces a temporal aspect to the scope of the design problem by investigating the life cycle potential of the process in terms of energy usage and waste generation.

Furthermore, the above are to be studied:

- in a multi-objective environment targeting the minimisation of the energy usage, the environmental impact and of course the cost
- employing a new process synthesis representation and methodology that is based on elementary physico-chemical phenomena.

Considering the complexity and the diversity of the above tasks, it becomes clear that the organisation of the various tasks in a coherent whole is a crucial issue in the development of the project. The basic elements of this framework involves:

a. Establishing the principles and the methodologies of the multi-objective environment.
b. Decomposing the overall synthesis project into manageable components.
c. Establishing an operation-based development of the whole synthesis project that combines a knowledge-based development of alternatives and preliminary screening and a mathematical-programming-based evaluation of the alternatives and determination of optimal configurations.

This report addresses the issues outlined above in some detail. In the second section the multi-objective environment issues are introduced and in the third section a decomposition of the problem is suggested and the design framework is presented.

4.1.1 A Multi-Objective Environment In Process Synthesis

Process synthesis is the generation of conceptual flowsheets. The steps involved in this activity include the identification of the potential chemical routes, e.g. the selection of the raw materials and the chemical recipe that leads to the

desired products, the development of alternative processing routes that conceptually drive the respective raw materials to the targeted product(s) and the selection among the developed processing routes the most preferred one.

As the conceptual design of a process fixes about the 80% of its total cost and it has a decisive impact on all aspects of the process performance it has long been recognised that it is essential to take into consideration at this early stage of the process'life, as many as possible, hopefully all, aspects of the multidimensional process performance. The key idea that shapes the way we are currently perceiving the process synthesis problem is that prevention is much more efficient than cure. It is much better to:

- design an energy efficient and integrated process than strive to heat integrate the already designed process

- prevent the generation of wastes than striving to minimise them via an end-of-the-pipe treatment

- create inherently safe and environmental friendly process operations than suffer the risk of human or ecological losses

- design a process that is flexible against the uncertainties over its resources, prices and demand of its products and raw materials, etc. than having to retrofit the design for every uncounted uncertainty

- design a process with a provision for its actual operation, e.g. its dynamic response and controllability than trying to tame it on line.

Attempting to capture the multi-dimensional nature of the process functions at the early synthesis/design level leads naturally to a multi-objective perception of the process synthesis task. However, as the objectives now sought at the process synthesis level are incommensurable, the whole concept of the optimal design looses its simple minded uniqueness and utopian appeal. The whole process synthesis procedure now acquires its natural dialectic quality and becomes the stage where all the real hard decisions have to be made. It is only fair after all that if someone wants to enrich in attributes his design decisions, attributes that may well be incommensurable, he has to trade at this point for the price that is to be paid in order to achieve the additional attributes.

As a result, the process synthesis problem has to be rephrased. What is to be delivered is not the best possible flowsheet, but a framework that will provide to the decision maker in a comprehensive and meaningful manner the trade-offs that are at stake in order to reach robust and knowledgeable design decisions. Elaborating a little on this last issue, it is useful to mention that in a single objective environment, the decision maker implicitly makes *a priori* a major decision: to ignore any other aspect in the synthesis process. A rather simplistic and biased trade off. The multi-objective environment to be employed in this project does not undertake any decision making that replaces the initial

indecision of the decision maker. Its scope is to defer the decision making action at a posterior phase where the synthesis project has evolved up to the state of providing the exact interaction between the various design objectives as this is mapped in specific design alternatives.

As in the single objective environment, the synthesis procedure maps the one dimensional design objective to a specific optimal process, in the multi-objective objective environment the process synthesis procedure maps the multiple design objectives to a set of design alternatives that represent the optimal trade off between the various objectives. This optimal trade off set is from the mathematical point of view, the exact mathematical solution of the multi-objective synthesis problem, just as the single optimal process is the mathematical solution of the single objective problem. And as this single optimal solution encompass an *a priori* taken decision, the optimal trade off set necessitates an *a posteriori* decision. The fundamental difference though is that whereas in the former case the decision maker is forced to a blind and implicit decision in a knowledge vacuum, in the latter case he has at his disposition the whole picture of exactly how much each objective is traded against any other and which design alternatives are implied in this trade off.

The optimal trade-off set is called the Pareto optimal solutions (alternatively termed non-dominated solutions, efficient set, or admissible set). The main property of the set of the Pareto optimal solutions is that for all solutions outside this set we can find a Pareto optimal one at which all objective functions are unchanged or improved and at least one is strictly improved. The problem of the formulation of a single optimality criterion problem from a number of essentially non-comparable elementary criteria was first treated by Pareto (1896).

Considering the general multi-objective optimisation problem to be stated as:

$$\begin{aligned} & \min \quad \mathbf{f}(\mathbf{x}) \\ \text{st.} \quad & \mathbf{g}(\mathbf{x}) \le \mathbf{0} \\ & \mathbf{h}(\mathbf{x}) = \mathbf{0} \\ & \mathbf{x} \in S \end{aligned} \tag{1.1}$$

the feasible region or decision space can be described by the set $X = \{\mathbf{x} \mid g_i(\mathbf{x}) \le 0, i = 1,...,m, h_j(\mathbf{x}) = 0, j = 1,...,p, \quad \mathbf{x} \in S \subseteq R^n\}$ and the criterion space, which is the image of X through the vector function $\mathbf{f}(\mathbf{x})$, can be denoted by the set $F = \{\mathbf{f}(\mathbf{x}) \mid \mathbf{x} \in X\}$ The essence of the difficulty to construct an optimality expression for (1.1) lies on the fact that it is no more possible to define a complete order in F as opposed to the scalar optimisation problem (N=1), where the natural order provides a complete order in F. Thus in (1.1), optimality is defined through a partial order, first introduced by Pareto (1896) according to the following definition:

Definition 1: A point $\mathbf{x}^*$ is said to be a non-inferior (Pareto optimal) solution of (MOP) if there does not exist any other $\mathbf{x} \in X$ such that

$$\mathbf{f}(\mathbf{x}^*) \leq \mathbf{f}(\mathbf{x}) \text{ and } f_i(\mathbf{x}^*) < f_i(\mathbf{x}) \text{ for some } i \in I_N$$

that is, a point $\mathbf{x}^*$ is considered to be non-inferior, if there does not exist any feasible point that improves one objective without degrading some other. The above definition establishes only a partial order, in the sense that it leaves incomparable the non-inferior solutions, e.g. $\mathbf{f}(\mathbf{x}^1)$, . $\mathbf{f}(\mathbf{x}^2)$ for which $f_i(\mathbf{x}^1) \geq f_i(\mathbf{x}^2)$, $i \in I_k \subseteq I_N$ and $f_j(\mathbf{x}^1) \leq f_j(\mathbf{x}^2)$, $j \in I_N \setminus I_k$

To address MOP the å-constraint method is going to be employed that transforms MOP to a multi-parametric scalar optimisation problem of the form:

$$\begin{aligned} & \min \quad f_i(\mathbf{x}) \\ st. \quad & \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \\ & \mathbf{h}(\mathbf{x}) = \mathbf{0} \\ & f_j(\mathbf{x}) \leq e_j, \; j = 1, N, j \neq i \\ & \mathbf{x} \in S \end{aligned} \qquad (1.2)$$

Algorithms and techniques for fully resolving this problem are currently available, especially for the bi-objective problem (or its equivalent single parametric one). The Pareto optimal solution set (line P_1-P_2-P_3-P_4-P_5-P_6-P_7) of a bi-optimisation problem is shown in Figure 1.1.

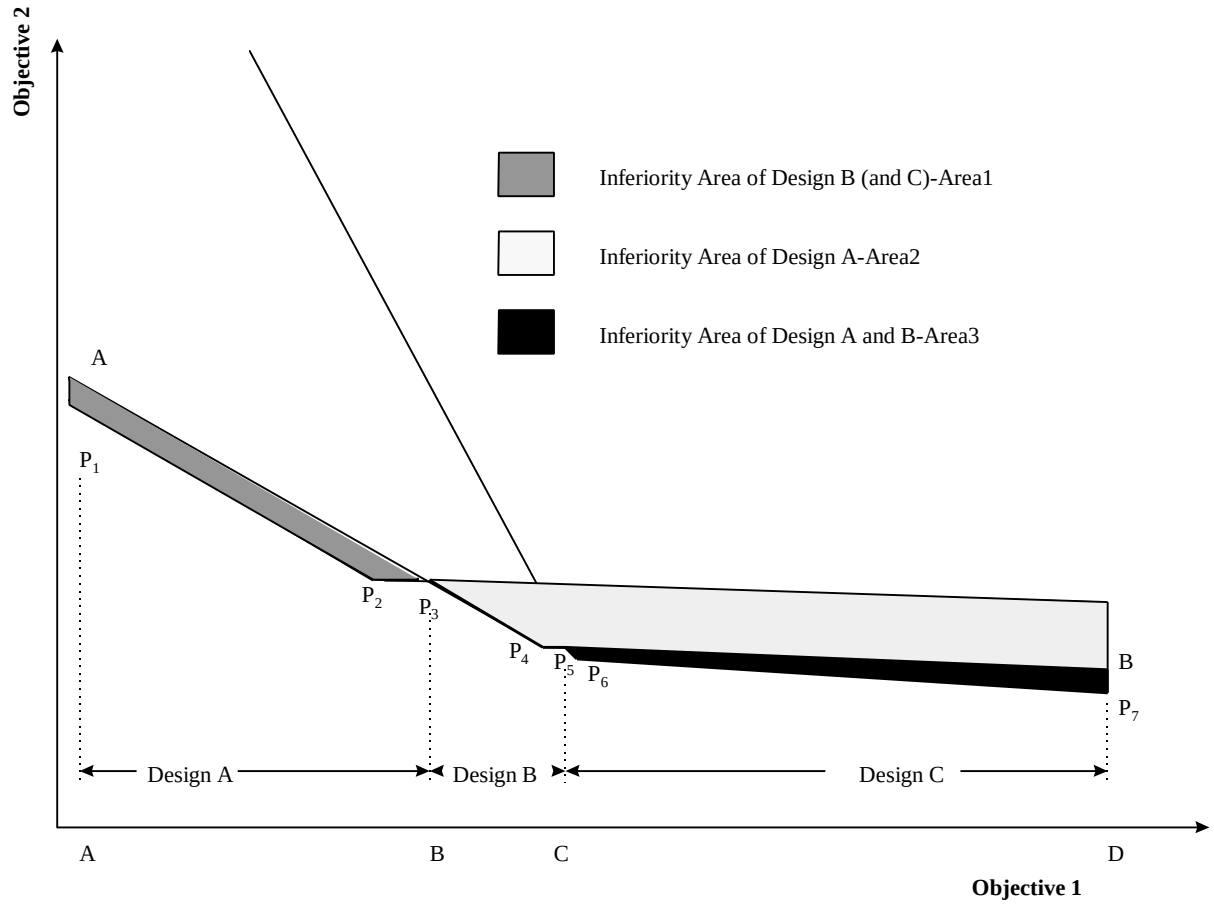


Figure 1.1. : Pareto optimal solutions of the a bi-objective optimisation problem.

The resolution of this parametric problem generally identifies regions over which a specific flowsheet structure is optimal (e.g. design A, B or C) and within each region (e.g. BC for design B) different realisations of Pareto optimal trade-offs is accomplished (line P_3-P_4-P_5) by the mere shifting the operational characteristics of this structure. Having though fully resolved problem 1.2, one can further proceed to obtain the full parametric solution of each of the Pareto optimal structures (e.g. line A- P_3-P_4-P_5-B for the design B) and assess the performance of the specific design at the whole range of the examined trading off between Objective 1 and Objective 2. By doing so, one can visualise the magnitude of inferiority of each structural solution outside its Pareto optimal range. This can be easily quantified in a metric of the form:

$$\int_S PO - Par(PO)_i \qquad (1.3)$$

where S is the range of parameterisation, PO is the Pareto Optimal solution along S (line P_1-P_2-P_3-P_4-P_5-P_6-P_7) and $Par(PO)_i$ is the full parametric solution of the i-th Pareto optimal solution (line A- P_3-P_4-P_5-B for the design B). Furthermore, a criterion for a most preferred solution can be then readily considered, by identifying as most preferred structure, the one with the best overall performance. This criterion can be explicitly stated as:

$$\Pr eferred \;\; Structure = \arg\left\{ \min_{Pareto\ solutions} \int_{S} PO - Par(PO)_i \right\} \qquad (1.4)$$

The term in the integral for Design A, as pictured in Figure 1.1, is Area2+Area3, whereas for Design B is Area1+Area3. Thus, for the example depicted in Figure 1.1 the use of the suggested criterion identifies Design B as the most preferred solution.

It has to be mentioned though that such a preferred solution selection, among the Pareto optimal ones, can only be viewed to have an advisory character. The major output of the multi-objective optimisation procedure is considered to be the full Pareto optimal set itself, that sets the ground for a knowledgeable decision making.

4.1.2 The Unified Framework

Problem Decomposition

The basic principle that shapes our approach in organising the various tasks undertaken in this project is the identification of a balanced compromise between a:

- decomposition/hierarchy of the various aspects and considerations of the process synthesis project and a

- centralised co-ordination that will keep track of the project evolution, it will at every stage be fully aware of the project status and will interact functionally with a human decision maker.

The backbone of the design framework, which is referred as process synthesis kernel, combines a non-monotonic variant of the means end Analysis technique and a superstructure optimisation method that is based on a multipurpose mass/heat transfer module representation framework. The issues that are functionally decomposed from this kernel include:

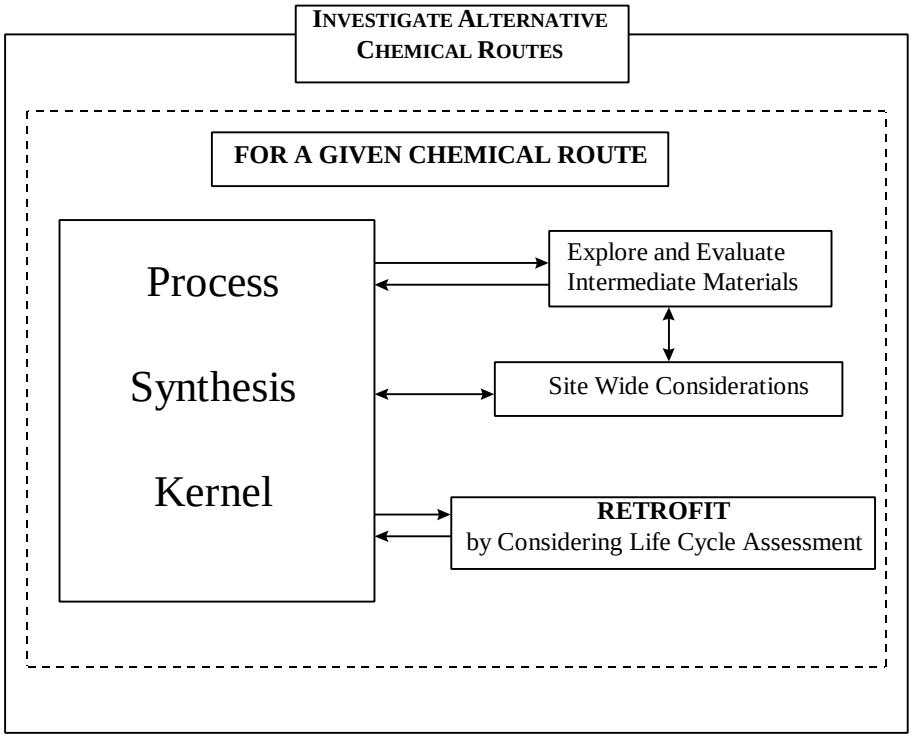


Figure 1.2: A first draft of the design framework.

1. The investigation of alternative raw materials/reaction paths that may suggest fundamentally different processes and they are to be compared and developed independently.

2. The selection of solvents, catalysts and intermediate process materials that can be set as independent tasks with predetermined scope (functionality requested from the materials) and selection criteria. The scope of the materials selection task is going to be determined by the synthesis kernel.

3. The life-cycle assessment that can be deferred to a latter stage. Based on a more schematic and concise representation of the developed flowsheet, the temporal aspects can be studied, possibly allowing for a conceptual retrofit of the grassroot design under development.

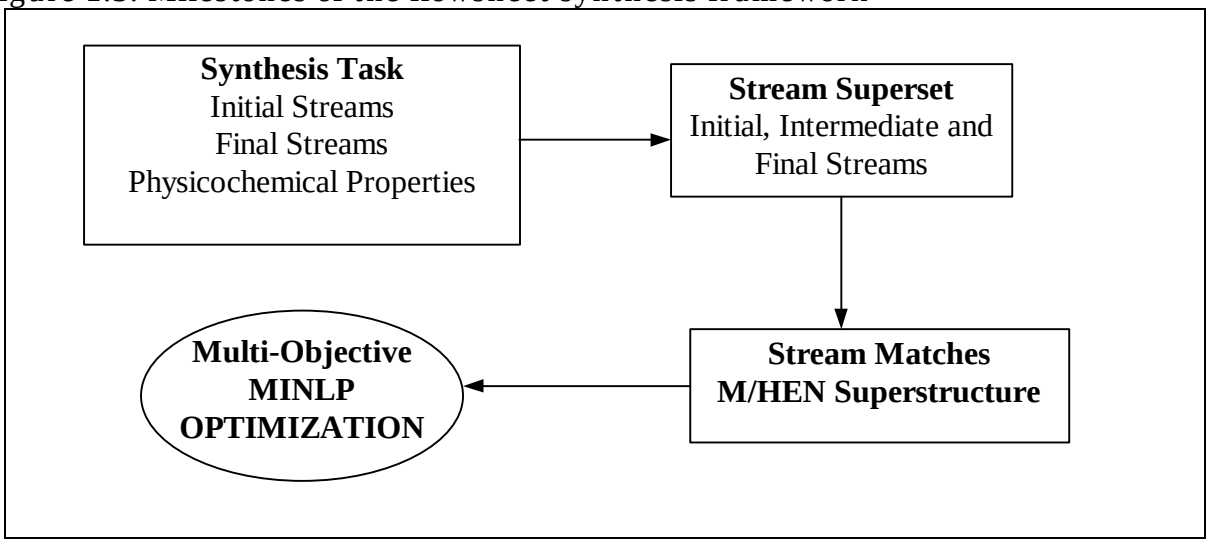
A first sketch of the design framework that results from the decomposition scheme outlined above can be seen in the following Figure 1.2.

Process Synthesis Kernel

In the operation-M/HEN generalised module based approach adopted in this project, it is assumed that the process synthesis activity commences with the specification of the initial and the final streams/materials (raw materials, products), it evolves to a stream superset that includes the intermediate streams/products (solvents, catalysts, etc.) and assigning the appropriate stream matches it builds the Mass/Heat Exchange Network Superstructure).

It then applies the developed criteria and optimises the M/HEN superstructure based on an operational based performance criterion and obtains the optimal path of the physico-chemical procedures that accomplishes the process synthesis task. The actual optimal unit structure is then left to be inferred from this procedural path. This is schematically shown in Figure 1.3.

Figure 1.3: Milestones of the flowsheet synthesis framework



Two important issues that are raised in order to transform this general plan to an actual, implementable, systematic and largely automated process synthesis procedure are the following:

1. The transition from the initial/final stream level of the process representation to the stream superset is actually a major synthesis task that includes important design decisions like the selection of the intermediate materials (e.g. solvents, catalysts) and the intermediate stream status, design decisions that essentially prescribe the process synthesis strategy that is to be adopted.

2. The transition from the stream superset to the M/HEN superstructure needs to be extensively explored so as to avoid including either physically meaningless or logically redundant matches without risking though to preclude matches that may eventually lead to novel and not intuitively suggestive unit configurations.

Addressing the issue of identifying the stream superset that includes all the intermediate process streams and states a Non-monotonic variant of the Means End Analysis methodology is suggested. According to the MEA methodology, the process synthesis problem is formulated as that of the recursive reconciliation of the differences between the raw materials, that is considered to be the initial state, and the desired products, that is considered to be the goal state.

The identification of the differences between two states/streams presumes

(a) a set of properties that characterises the pertinent streams that includes the molecular identity of the species present in the streams, the amount of the species involved, the composition or purity of the materials, the thermodynamic phase(s), the temperature, pressure, etc., e.g. all the attributes that characterises completely and uniquely a process stream.
(b) a hierarchy in this list of attributes that sets the order in which the differences are eliminated. Thus it is conventional practice to consider as first in this property list the molecular identity and then the species composition. Having set this order, the MEA procedure naturally identifies first the reactor and then the separator operators. The scheme is refined and enriched as the MEA proceeds lower in the stream properties list and/or examines the preconditions and post conditions of the applied operators.

The elimination of the identified difference is achieved through the application of an appropriate operator.

In the monotonic application of the MEA this step includes

(a) Search for an operator that eliminates the identified difference.
(b) Check the preconditions of each candidate operator and if all preconditions are satisfied apply it and pose its post-conditions and none of the available operators have their preconditions satisfied then backtrack and restart (opportunistically) alternative operator sequences.

In the non-monotonic variant that is suggested, the identification of a violated precondition prompts a MEA task that attempts to eliminate the difference between the current state and the desired precondition. Thus the algorithm proceeds by identifying recursively the operator that eliminates the differences between the current state and the determined preconditions and between the preconditions and the goal state.

The need for intermediate material usage reveals naturally in the course of this difference elimination procedure and can be used effectively to guide the material selection part of the project by identifying the properties and the functionality of the materials needed and assigning the proper material selection tasks.

The non-monotonic variant of the MEA methodology that is suggested has the following distinguishing features:

1. Goal-driven approach: It always starts from a desired goal state and tries to identify the requisite operations that will achieve it.
2. Constraint posting without backtracking: Instead of backtracking when a constraint violation is detected, the non-monotonic variant attempts to find an operator that would negate the violated preconditions and forces this operation to be applied before the operation that causes the impasse. The operator that poses the precondition violation, negates, prevents or undoes one or more of the process synthesis goals, is called a Clobberer. On the other

hand, an operator that rectifies, the preconditions' violation caused by the Clobberer is called Non-monotonic White Knight. The success of any non-monotonic planning methodology lies in its ability to identify these Clobberers and White Knights without having to resort to exhaustive generate-and-test approach. Once these operators have been identified, the Process Synthesiser must ensure that whenever a Clobberer is identified in the plan, an accompanying White Knight is present.

3. Generator of partial flowsheets: Non-monotonic synthesis generates partially specified flowsheets where a certain amount of information is not bound to specific values. Partial flowsheets are abstractions, which can represent large sets of flowsheets and can lead to efficient representations and search strategies.

At the end of this procedure a set of intermediate streams/ materials/ operations is determined. At this point, the operators can be removed and the specified flowsheet can retreat to an abstract construct of initial-intermediate-final streams, that is the stream superstructure of the M/HEN generalised module methodology. This abstraction is going to link the two methodologies in a coherent and unified methodology. It is important to note at this point the following:

1. Although a significant amount of information is negated by removing the operators from the NM-MEA suggested flowsheet(s), most of the engineering knowledge that has been already employed in terms of the material usage and the basic synthesis strategy is retained within this stream superset.
2. Although retaining all essential engineering knowledge employed, this conceptual retreat, allows a renewed truly combinatorial examination of the processing alternatives that may result to the postulated stream superstructure.
3. The shifting from the streams/operators structures to the streams M/HEN modules superstructure is functionally coherent as there is a common conceptual basis between the notions of the *elementary module* and the *operator*.
4. The postulation of the stream matches can now proceed in a knowledgeable manner so as to exclude redundant matches and reduce the problem's dimensionality. The ground of this last argument lies on the fact that as the stream superset is not arbitrarily postulated but is the abstraction of a knowledge based engineering artefact, it provides a solid basis for selectively allowing combinatorial alternatives.

Overall, the NM-MEA methodology contribution can be seen as that of identifying, in a systematic, knowledge-based framework, a set of realisable intermediate states (rather than actual flowsheets) that provides in a comprehensive way a knowledge-justified basis for the enumerative and combinatorial evaluation and selection methodologies of mathematical programming.

Enriching Figure 1.3, the process synthesis kernel is structured as it is shown in Figure 1.4. The steps in the process synthesis approach suggested can be summarised as follows:

(a) Employ a non-monotonic variant of the means end analysis technique, to develop a preliminary design with potential alternative paths.
(b) Remove the operators postulated in the previous step to retreat to a stream superset that includes the intermediate streams/products. (solvents, catalysts, etc.)
(c) Assign the appropriate stream matches and builds the Mass/Heat Exchange Network Superstructure.
(d) Employ MINLP optimisation techniques to deduce the optimal flowsheet configuration.

It is expected that the application of this platform on the case studies that are to be provided from the industrial partners is going to prove its validity and that the feedback from this application will help it evolve to a powerful methodological framework.

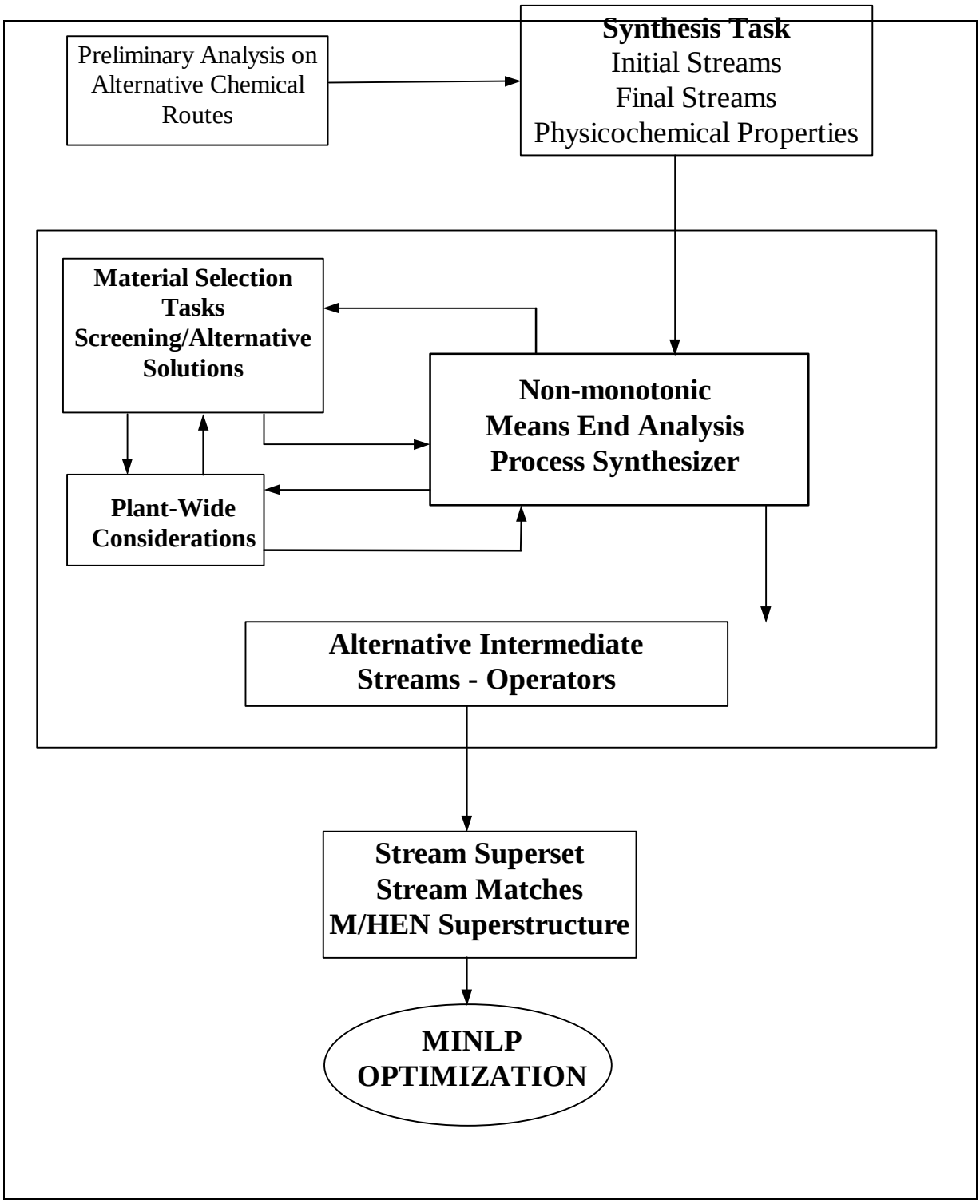


Figure 1.4. :Schematic representation of the synthesis kernel

4.2 Task [T2]: Synthesis of Energy Efficient Processing Routes and Schemes

Work in this task has addressed: (a) the validation and refinement of the proposed mathematical model for the synthesis of energy efficient process systems, based on a mass/heat transfer modular representation framework; and (b) the link with physical properties based on thermodynamic insights.

4.2.1 Mathematical Model for Mass/Heat Exchange Module

The Generalised Modular Representation framework for process synthesis based on mass / heat transfer principles has been developed. The underlying mathematical model to describe mass and heat transfer within the building block of the proposed modular superstructure of process alternatives, i.e. the mass / heat transfer module (Figure 2.1) has been revised, validated and enhanced.

Modelling of mass transfer has been generalised and the assumption of pre-postulated mass transfer direction for each component of interest is relaxed. Variable mass transfer direction is assumed for each component in each module and this is optimized based on driving force and equilibrium constraints.

The proposed model is validated simulating a separation system for a ternary and a four-component mixtures and with the synthesis of a separation system for a four-component mixture, and is compared to the conventional tray-by-tray distillation column model.

4.2.1.1 Description of the mathematical model

Mass and heat transfer within a mass/heat exchange block (Figure 2.1) is described by:

- Mass balance for each component around the block, including possible reactive mass transfer.
- Energy balance.
- Phase-definition constraints for the exchanging streams, at the inlet and the outlet of the module.
- Driving force constraints that ensure feasible mass transfer according to temperature and pressure conditions for each component.

If a component is transferred from the "rich" to the "lean" side of the module:

$$g_1 = f_R^{in} x_{R,c}^{in} - f_R^{out} x_{R,c}^{out} \geq 0 \quad \Rightarrow \quad g_2 = K_{R,c}^{in} x_{R,c}^{in} - x_{L,c}^{out} \geq 0$$
$$g_3 = K_{R,c}^{out} x_{R,c}^{out} - x_{L,c}^{in} \geq 0 \qquad (2.1)$$

otherwise:

$$g_1 = f_R^{in} x_{R,c}^{in} - f_R^{out} x_{R,c}^{out} \leq 0 \quad \Rightarrow \quad g_2 = K_{R,c}^{in} x_{R,c}^{in} - x_{L,c}^{out} \leq 0$$

$$g_3 = K_{R,c}{}^{out} x_{R,c}{}^{out} - x_{L,c}{}^{in} \leq 0 \qquad (2.2)$$

where f, x and K are total stream flows, molar fractions and equilibrium constants respectively. In general, transfer direction of each component within each mass/heat transfer block is also optimized including:

$$g_1 g_2 \geq 0$$
$$g_1 g_3 \geq 0$$

Mixed integer optimization techniques are employed to avoid the highly non-linear, non-convex constraints described above. A binary variable is introduced to denote the mass transfer direction for each component in each mass/heat transfer block:

$yt_{c,i}$ = 1, when c is transferred from "rich" to "lean" side in i block
0, otherwise

Then, mass transfer is sufficiently modelled by:

$$\begin{aligned} g_{1,i,c} - yt_{c,i} U &\leq 0 \\ -g_{1,i,c} + (1 - yt_{c,i}) U &\leq 0 \\ -g_{2,i,c} + (1 - yt_{c,i}) U - (1 - y_i) U &\leq 0 \\ g_{2,i,c} - yt_{c,i} U - (1 - y_i) U &\leq 0 \\ -g_{3,i,c} + (1 - yt_{c,I}) U - (1 - y_i) U &\leq 0 \\ g_{3,i,c} - yt_{c,i} U - (1 - y_i) U &\leq 0 \\ yt_{c,i} + y_i &\geq 1 \end{aligned}$$

where y_i denotes the existence of i module within the overall MINLP synthesis problem.

4.2.1.2 Examples

a) Separation of ternary mixture in 20 mass/heat transfer modules, simulating a distillation column.

An ideal ternary mixture of n-hexane, n-heptane and toluene is studied. A conventional distillation column is simulated by 20 modules/trays. One process feed and two products are considered (see Figure 2.2). The total pressure of the system is assumed 1 atm. Two products are considered. Maximization of separation efficiency and minimization of operating cost for constrained product compositions (i.e. of hexane concentration in the top product and toluene concentration in the bottom product) are studied.

The resulting separation profiles for the 20 mass/heat exchange blocks show the same trends as the profiles based on a tray-by-tray equilibrium model (Figures 2.3 and 2.4), proving the sufficiency of the proposed model to describe mass and heat transfer for the case of ideal separations. Note, that as a mass/heat exchange block can correspond to a set of trays, we observe sharper increase or

decrease in the concentrations of each components per module and better separation, limited only by thermodynamic conditions of the feed stream and product streams.

b) Separation of 4-component mixture in 20 mass/heat transfer modules, simulating a distillation column.

The separation of an ideal mixture of n-hexane, benzene, n-heptane and toluene in 20 modules, simulating a distillation column is studied, for maximum separation efficiency and minimum operating cost and constrained product compositions (see Figure 2.5).

The separation profiles for both cases are illustrated in Figures 2.6 and 2.7. Note again, that although basic separation trends and limitations are captured in the Mass/Heat Exchange Model, tray details are lost and sharper profiles are achieved. This implies that the Mass/Heat Exchange Network representation framework is sufficient to describe physico-chemical phenomena that drive a process and their limitations. Detailed design and evaluation of unit operations, however, involves further developments.

c) Synthesis of Separation System for a 4-component mixture.

The separation of a n-hexane/benzene/n-heptane/toluene mixture is studied (see Table 2.1). Two products are of interest, one rich in n-hexane and one rich in toluene. A mass heat exchange superstructure, involving 20 mass/heat exchange modules and all possible interconnections between exchanging streams, is optimized. The initial liquid feed is assumed to enter mixers prior to exchanger rich sides and superstructure coolers. A heater (total reboiler) is assigned to each lean inlet of the superstructure modules and a cooler (total condenser) to each rich inlet of the modules.

A total cost is minimized accounting for:

- operating cost for heaters and coolers
- fixed cost for each module, denoting an estimation of capital cost.

The synthesis problem is an MINLP, involving 5305 rows, 4133 continuous variables, 2720 binary variables and 15860 non-linear terms, is solved employing Generalised Benders Decomposition (Geoffrion, 1972) as applied in General Algebraic Modelling System (GAMS) modelling language. Only 20+80 binary variables are actually required to denote the existence of mass/transfer and heat exchange modules and mass transfer directions of the components. The rest are structural variables that are utilised to simplify the resulting NLP sub-problems. Logical integer constraints on these variables reduce significantly combinatorial complexity.

Feed Data

Flowrate	n-Hexane	Benzene	n-Heptane	Toluene	Temperature

(kmol/s)					(K)
50	0.3	0.2	0.2	0.3	355

Cost Data

Cooling Water Cost ($ / kWyear)	Steam Cost ($ / kWyear)	Fixed Cost per Block ($ / year)
26.19	137.27	1000

Product Specifications

Hexane-rich product	Toluene-rich product
$f \geq 10$ $x_{hexane} \geq 0.97$	$f \geq 10$ $x_{toluene} \geq 0.90$

Table 2.1: Synthesis Example

The optimal solution is illustrated in Figure 2.8. Alternatively, the conventional separation scheme for a 4-component mixture is illustrated in Figure 2.9, featuring a higher cost. It is interesting to see that the same model can result in very different separation schemes without having pre-postulated any particular structural or separation schemes.

4.2.2 Integration with Physical Properties

Structural, chemical and physical properties of pure components and mixtures are closely related to the separation process principles since differences in the values of properties among the components of the mixture to be separated are exploited by the separation techniques. While some properties may depend on temperature (T) and pressure (P), the condition of operation of many separation techniques may also be defined in terms of T and P. Thus, the dependence of the properties on these state variables not only helps to select the appropriate operating ranges for T and P, but also, to determine the process sensitivities (which are of importance when process operation/control need to be considered). Since most process streams contain binary or multi-component mixtures, the dependence of a property on the component identities and their composition also play an important role in the choice of the condition of operation. Consequently, the differences (or property ratios) in the values of the properties identify a separation technique, the values of T, P and/or composition at which a sub-set of properties attain desirable values, provide good estimates of the condition of operation of the separation technique, while, the rates of changes of the same properties with respect to T, P and composition influence the control and operation of the process.

An algorithm has been developed based on the principles described above. It is illustrated with a simple example consisting of a binary azeotropic mixture (also found in the methanol case study). Five possible separation alternatives exist if only separation through vapour and liquid phases (any combination) is considered. These alternatives are based on the following - homogeneous system (formed with a solvent), binary heterogeneous azeotrope, heterogeneous system (formed with a solvent), pressure sensitive azeotrope, azeotrope disappearing at a limiting pressure. For each of these cases, different separation techniques can be employed. For homogeneous systems, it is possible to employ extractive distillation, liquid-liquid extraction and supercritical extraction. For binary heterogeneous azeotrope, conventional distillation followed by separation of the azeotrope in a decanter is feasible (solvents are not needed in this case). For heterogeneous systems, azeotropic distillation, liquid-liquid extraction and supercritical extraction are possible alternatives. For pressure sensitive azeotropes, the desired separation can be achieved in configurations of two conventional distillation columns. Finally, if the azeotrope disappears at a certain temperature, separation in a single conventional distillation column at a specified pressure may become feasible. In the case of the solvent based separations, the choice of the solvent and the resulting phase diagrams and phase equilibrium computations (bubble-point/dew-point) provide the necessary estimates for the condition of operation in terms of operating ranges for T and P, and, product compositions (specifications). In the case of pressure-based distillation column configurations, the phase equilibrium computations (bubble-point/dew-point) at the selected pressures provide the necessary estimates for the conditions of operation. The algorithm involves the following steps :

1. Perform a mixture analysis in order to determine the binary and ternary azeotropes and their pressure dependence.
2. Determine the candidate solvents for the separation of the binary azeotropic mixtures.
3. Classify the binary and/or ternary mixtures (with solvents).
4. If the binary azeotrope is pressure sensitive or is heterogeneous, select separation without solvent as an alternative. Otherwise, select solvent-based separation as the only alternatives (if suitable solvents can be found).
5. For separation without solvents, choose a two conventional distillation column configuration as an alternative if the azeotrope location changes with pressure. Choose a separation by one conventional distillation column if the azeotrope disappears at a specific pressure. Choose a configuration consisting of a conventional distillation column and a decanter if a heterogeneous binary azeotrope is found.
6. If suitable solvents can be found, select the corresponding solvent based separation (extractive distillation, azeotropic distillation, liquid-liquid extraction and supercritical extraction). Note that the selection of the solvent determines also the separation technique.
7. For each selected separation technique, determine the condition of operation. In the case of pressure sensitive operation, determine bubble-point/dew-point temperatures at the selected pressure. In the case of separation with a decanter, determine the T and/or P at which the azeotrope splits into two liquid phases. In the case of solvent-based separation, the ternary phase diagrams provide the estimates for T, P and product compositions.
8. Validate the initial synthesis (separation process configuration) and design (operation conditions and product specification) through rigorous simulation.

The integrated algorithm for synthesis and design has been applied to determine the initial design for the methanol production case study. Application of the above algorithm also requires a number of computational tools. In the next section, the integrated computational tools are described.

The computer program package developed at DTU for process synthesis and design consists of three types of programs: (a) Those that perform various types of computations, such as predictions of properties, computation (simulation) of single and multiple stage separations; (b) Those that are related to the knowledge base, consisting of component data banks (with pure component properties), group-model parameters, separation feasibility matrix; and (c) Those that generate graphical output, such as phase diagrams for analysis.

a) Knowledge Base

i) Information related to components: This comprise experimental data of pure component properties from physical properties data bank for more than thousand compounds, group model parameters for prediction of pure component and mixture properties, correlations for property prediction etc.

ii) Information related to separation techniques: This includes information on suitable separation techniques for specific mixtures, and suitable solvents for specific solutes, suitable external agents for separation of specific compounds or classes of compounds, information about suitable conditions of operation and separation factors for external agents, information about suitable separation techniques for bulk/dilute and high purity/low purity separations, information of separation feasibility indices in the form of a separation feasibility matrix.

b) Mixture Analysis

Program 1: Mixture analysis and thermodynamic model selection
Based on the identity of the mixture components, temperature, pressure and composition of the components, the program identifies the mixture type (for example non-ideal, polar-associating mixture) and proposes a suitable thermodynamic model for prediction of phase equilibrium and properties.

Program 2: Reactivity predictions
Based on the identity of the mixture components, temperature and pressure, and pure component properties, such as Gibbs free energy of formation, heat of formation, entropy of formation and the ideal heat capacity, simultaneous chemical and phase equilibrium is predicted, (Castier et al., 1988) and the program computes the converged mole fractions in all (stable) phases.

Program 3: Identification of azeotropes
This program calculates binary and ternary azeotropic points, bi-nodal curves as a function of temperature, corresponding equilibrium vapour line and residue curves. The information required is the identity of the components, the property prediction model and a specified pressure.

Program 4: Prediction of liquid-liquid phase split
Binary solubility predictions are computed based on the identity of the components in the binary pair, the temperature and an initial estimate of the concentration of the components in the different phases.

Program 5: Identification of eutectic points
The program predicts solid-liquid equilibrium and eutectic points for binary mixtures. The identity of the components, heat of fusion, melting points and physical property model must be specified.

Program 6: Solubility prediction
Solubility of liquids is predicted based on liquid phase activity coefficients with different thermodynamic models. The information necessary is the identity of the components and the mixture temperature. The mutual solubilities and aqueous solubilities are predicted with infinite dilution coefficients based on modified UNIFAC (Larsen et al., 1987) and the UNIFAC model for aqueous systems (Chen et al., 1992) at T=298 K. The UNIFAC parameters for aqueous systems have been updated/added to the computational tools for the purpose of

this work. For gas solubilities and solubilities in supercritical solvents, the MHV2 model is employed (Dahl et al., 1991).

c) Binary ratio matrix and separation technique identification

Program 7: Binary ratio matrix and separation technique identification
Pure component properties of more than a thousand components have been extracted from the physical properties data base for quick and easy access to the binary ratio matrix. Rules have been added for computation of the binary ratio matrix where the only information required is the identity of the compounds. In addition, rules for separation technique identification have been implemented.

d) Identification of Mass Separating Agents

Program 8: Prediction of solubility parameters and solubility
A program has been developed for computation of solubility parameters and molar volumes by group contribution. In addition, the program predicts solubility based on solubility parameters, and several important pure component properties for design of solvents. Also, the program predicts whether two liquid phases are possible or may not exist.

e) Estimation of conditions of operation

Program 10: Computation of phase diagrams
Programs for prediction of phase diagrams are available, such as bubble point curves, dew point curves phase envelopes. The information required is the identity of the components, the pressure and/or temperature.

f) Flowsheet Analysis and Optimization

Program 11: Steady state simulator
A steady state simulator (Perregaard, 1992) with several different unit options is available as a computational/analysis tool to verify the process flowsheets generated. Separation units such as supercritical extraction, multiphase flash operation, liquid-liquid extraction, distillation, absorption, gas separation membranes, stripping, etc., are available for process simulation. With process simulation the generated flowsheet is analysed. The effect of recycle streams, feed location, reflux and number of stages on the product purity is analysed. Pumps, valves and/or compressors are included if necessary.

Program 12: Optimization routine
Programs for Mixed Integer Non-linear Programming (MINLP) optimization are available at Imperial College.

In addition to the programs mentioned above, programs are also available for accurate estimation of pure component properties through group-contribution prediction techniques. This is useful for determining properties of compounds for which no experimental data is available.

4.3 Task [T3]: Site Wide and Operational Considerations – Case Study 2 (Task [T6]): Optimal Scheduling in Paper Converting Industry

The Process Design Laboratory of the Department of Chemical Engineering at Åbo Akademi University has participated in the IDEES-project with the main focus on tasks considering the industrial problems at WalkiWisa Wisapak. Due to the general complexity of the problems, several scientific aspects have been critical to the problem treatment. Therefore, different transformation strategies, mixed integer non-linear programming (MINLP) methodology development and site-wide and operational issues with special weight on the environmental and energy aspects have been studied. In parallel, the development of an already existing scheduling tool, the Wisatrim, has been carried on at the paper converting mill.

Nomenclature for this section

B_{max}	The maximum possible width of a pattern (≈ the raw paper width)
B_j	Width of a cutting pattern
m_j	Number of times the cutting pattern j is used
y_j	A binary variable to determine if pattern j is used
c_j	The cost of a knife change of pattern j
C_j	The cost of the raw paper for pattern j
P_m	Energy consumption of a machine (kW)
l_j	Length of a cutting pattern/product reel
v_m	Speed of a coating machine/slitter
t_j	Time for a knife change
f	A factor that determines the value of over-production

In order to get better insights into the problem area, a brief introduction of the paper converting and its main scheduling problems is given in the following.

4.3.1 The Paper Converting Industry

An integrated paper mill can be roughly divided into three main production units. In one unit pulp is produced. A pulp mill uses as input some kind of wood or fibrous raw material and produces pulp for the paper machines.

The second production unit is the paper mill. A paper mill can be a combined pulp & paper mill or located near a pulp mill and only produce the paper and thus, roughly consist of a set of paper machines. In the paper machines the pulp is processed to form wide raw paper reels width widths varying between 3000 and 8000 mm. The speed of a paper machine varies from 1000 to 2500 meters per minute.

The raw paper is passed to the third unit, the paper converting mill. In a paper converting mill, the raw paper from the paper mill is further processed in

various ways. Normally the paper mill deliver some standard widths to the paper converting mills. The widths are normally varying from 1500 mm to 3500 mm, depending on the machinery.

The raw paper can be processed in several different ways in a paper converting mill. The raw paper can be cut, printed, coated, glued and finally packed for delivery. A typical paper converting mill, like the WalkiWisa Wisapak, has about 600 different products to produce for different customers. Customers are for instance mills that produce paper sheets for photocopying and laser printing. The scheduling of the operations in a paper converting mill is a huge task and has been done so far by a full-time scheduler. Thus, there is a lot of profits to expect if even a part of this scheduling could be done by some kind of mathematical programming optimization. One of the most difficult tasks in the scheduling of a paper converting mill is to determine how to do the cutting of raw paper reels in an optimal way.

The cutting has traditionally been scheduled by a group three employees. The scheduling has also been done using some heuristic programs or some specific programs made at the mill. Even linear programming (LP) has been used to tackle this critical problem. Because of the integer nature of the cutting problem, the LP-methods have, however, given poor results and have, thus, not been competitive to the manual planners in long time perspective.

4.3.2 The Trim-Loss Problem

The actual problem is to minimize the paper waste that appears when some arbitrary wide paper reels, specified by the customer are cut from raw paper reels, more or less, specified by the paper mill. One fact is that the incoming raw paper width cannot be adapted to the widths ordered by the customers and produced by the paper converting mill. The material that forms the paper waste could be used to produce product reels and includes therefore an economical loss. Besides the economical loss, there are some environmental aspects: the energy consumption and the waste treatment problem. If the average waste of 4-5% can be reduced to 2%, then the energy demand for the production can directly be reduced by at least 2-3%. This is due to, for instance, a reduced production time.

A more effective production also reduces the waste treatment problem. In the paper converting mill the paper is often coated with polyethene or some other plastics and printed in different colors. Because of the usage of different chemicals, most of the waste cannot be recycled to the pulp mill. Furthermore, a part of the waste may not be burned either because of harmful atmospheric emissions. Thus, the minimization of the waste, the trim loss, seems to be a good strategy to minimize both production costs and harmful environmental impacts.

In the trim-loss problem, the main objective is to reduce the paper waste (spill) that appears during the slitting process where a jumbo reel is cut into product reels. The optimization can be done with different heuristic methods but here a mathematical programming approach is considered in order to obtain the global optimal solution.

4.3.2.1 The Basic Formulation

The trim loss problem is basically a non-convex MINLP problem owing to bilinear demand constraints. The existence of integer variables makes the problem very hard to solve because of the huge combinatorial field. Considering the printing and coating processes at a paper converting mill together with the trim-loss approach seems to raise very complicated problems and therefore it is proposed to keep the trim loss problem as a separate problem.

In the following a formulation for the trim loss problem is given according to Harjunkoski et al. (1996).

$$\min_{m_j, n_{ij}, y_j} \left\{ \sum_{j=1}^{J} c_j \cdot m_j + C_j \cdot y_j \right\} \tag{1}$$

subject to

$$\sum_{i=1}^{I} n_{ij} \cdot b_i - B_{\max} \le 0 \tag{2}$$

$$-\sum_{i=1}^{I} b_i \cdot n_{ij} + B_{\max} - \Delta_j \le 0 \tag{3}$$

$$\sum_{i=1}^{I} n_{ij} - N_{\max} \le 0 \tag{4}$$

$$y_j - m_j \le 0 \tag{5}$$

$$m_j - M_j \cdot y_j \le 0 \tag{6}$$

$$j = 1, \mathrm{K}\ , J$$

$$n_{i,order} - \sum_{j=1}^{J} m_j \cdot n_{ij} \le 0 \tag{7}$$

$$i = 1, \mathrm{K}\ , I$$

$$m_j, n_{ij} \in Z^+$$

$$y_j \in \{0,1\}$$

Because of the bilinear inequality (7), the problem is both nonlinear and non-convex. The objective minimizes the total number of cutting patterns and the number of pattern changes. The problem is solved with both linear and non-linear methods in Harjunkoski (1997a)

The trim loss problem has been an essential research topic, since it includes both numerical and computational difficulties. The existence of integer variables makes the problem very hard to solve because of the huge combinatorial field. While an expansion of the trim loss problem to cover a bigger field seems to be as good as impossible at this stage, it is proposed to

keep the trim loss problem as a separate problem. The work has been focused on investigating different methods for handling bilinearities appearing in scheduling problems, especially in trim-loss problems. In trim-loss problems the bilinearities are very tough due to the fact that both variables in the bilinear expressions are integers. The linear transformations are working, but give rise to a dramatic increase in the number of both variables and constraints.

4.3.2.2 Convex transformations

The problem is fully linear except for the bilinear demand constraint (7). Therefore the key issue is how to rewrite the terms $m_j\ n_{ij}$. There are several ways to transform or parameterize the non-convex problem into linear form. The main drawback for the linear transformation strategy is the large number of extra constraints and continuous variables. The parameterization strategy results in a formulation with a few constraints but many extra integer variables.

In the following comparison 5 different linear (MILP) transformations are used. Transformation 1 includes a binary representation of m_j and definition of slack-variables s_{ijk}. Transformation 2 is similar but here the variable n_{ij} is represented by binary variables. In the transformation 3, n_{ij} is parameterized by generating all possible cutting patterns. Transformation 4 includes parameterization of m_j which is a bit more difficult than the previous one. The last transformation 5 presents a special case of transformation 4 where all m_j variables are set to be equal to 1.

A number of convexification methods may also be applied. Generally, the convex formulations need fewer extra constraints and continuous variables than the linear strategies and no extra integer variables as is the case with the parameterization methods. Thus, the convex transformation could be expected to result in formulations easier to solve especially for larger-scale orders. This creates an interesting problem, where the integer search space is reduced with the expense of more complex non-linear functions, that could in principle be used as a benchmark for the performance of MINLP algorithms.

The basic principle for the convex transformation is to first expand the bilinearity in the demand constraint

$$m_j \cdot n_{ij} = (m_j + t)(n_{ij} + t) - t \cdot (m_j + n_{ij}) - t^2 \tag{8}$$

In the following text, the translation constant $\tau = 1$ is used for simplicity. The second step is to substitute the bilinear term in the original demand constraint

$$n_{i,order} - \sum_{j=1}^{J}(m_j + 1)(n_{ij} + 1) + \sum_{j=1}^{J}(m_j + n_{ij}) + J \le 0 \tag{9}$$

The transformations require that m_j and n_{ij} are defined as

$$m_j = \sum_{l=1}^{L_j} b_{jl} \cdot l \quad n_{ij} = \sum_{k=1}^{K_i} b_{ijk} \cdot k \tag{10}$$

$$\sum_{l=1}^{L_j} b_{jl} \le 1 \quad \sum_{k=1}^{K_i} b_{ijk} \le 1 \tag{11}$$

In two of the following transformations a variable r_{ij} needs to be defined to make the negative bilinear terms positive. The variable r_{ij} is the opposite value of n_{ij} and is defined as

$$r_{ij} = N_{j,\max} - n_{ij} \tag{12}$$

The convex transformations are presented very briefly here. Further details can be found in the references. In the following, only the transformation itself and the resulting convex demand constraint are presented.

6. Exponential transformation

$$m_j + 1 = e^{M_j} \quad r_{ij} + 1 = e^{R_{ij}} \tag{13}$$

$$n_{i,order} - J + \sum_{j=1}^{J} e^{M_j + R_{ij}} - \sum_{j=1}^{J} \left((N_{\max} + 1) \cdot \sum_{l=1}^{L_j} b_{jl} \cdot l + \sum_{k=1}^{K_i} b_{ijk} \cdot k \right) \le 0 \tag{14}$$

7. Square-root transformation

$$m_j + 1 = \sqrt{M_j} \quad n_{ij} + 1 = \sqrt{N_{ij}} \tag{15}$$

$$n_{i,order} + J - \sum_{j=1}^{J} \sqrt{M_j \cdot N_{ij}} + \sum_{j=1}^{J} \left(\sum_{l=1}^{L_j} b_{jl} \cdot l + \sum_{k=1}^{K_i} b_{ijk} \cdot k \right) \le 0 \tag{16}$$

8. Logarithmic and square-root transformation

$$m_j + 1 = \sqrt{M_j} \quad n_{ij} + 1 = \ln N_{ij} \tag{17}$$

$$n_{i,order} + J - \sum_{j=1}^{J} \sqrt{M_j} \cdot \ln N_{ij} + \sum_{j=1}^{J} \left(\sum_{l=1}^{L_j} b_{jl} \cdot l + \sum_{k=1}^{K_i} b_{ijk} \cdot k \right) \le 0 \tag{18}$$

9. Inverted transformation

$$m_j + 1 = \frac{1}{M_j} \quad r_{ij} + 1 = \frac{1}{R_{ij}} \tag{19}$$

$$n_{i,order} - J + \sum_{j=1}^{J} \frac{1}{M_j \cdot R_{ij}} - \sum_{j=1}^{J} \left((N_{\max} + 1) \cdot \sum_{l=1}^{L_j} b_{jl} \cdot l + \sum_{k=1}^{K_i} b_{ijk} \cdot k \right) \le 0 \tag{20}$$

10. Modified square-root transformation

$$m_j = \sum_{l=1}^{L'_j} 2^{l-1} \cdot b_{jl} \tag{21}$$

$$n_{i,order} + J - \sum_{j=1}^{J} \sqrt{M_j \cdot N_{ij}} + \sum_{j=1}^{J} \left(\sum_{l=1}^{L'_j} 2^{l-1} \cdot b_{jl} + \sum_{k=1}^{K_i} b_{ijk} \cdot k \right) \leq 0 \tag{22}$$

This strategy also requires slack-variables and some slack-constraints

4.3.2.3 A Numerical Example

The following numerical example can be found in Harjunkoski et al. (1997b). Some improvements can be observed when comparing the old optimization results with the new ones. A maximum order limit has been used for problem reduction.

Table 1. Example order

Product (i)	Width (b_i)	Number ($n_{i,order}$)	Maximal production
1	330	8	10
2	360	16	18
3	380	12	14
4	430	7	9
5	490	14	16
6	530	16	18

The MILP problems (1-5) have been solved with CPLEX-4.0 and the MINLP problems (6-10) with 'mittlp' that implements the Extended Cutting Plane algorithm. Some problem information and optimization results are presented in the following table.

Table 2. The optimization results

Method	Variables (I/B/C)	Constraints (L/NL)	Nodes/ECP-iterations	CPU-time (s)
1	36/23/120	408/-	439	10.55
2	6/88/144	366/-	179	1.72
3	51/51/-	59/-	1560	33.38
4	282/47/-	201/-	541	8.60
5	102/18/-	265/-	128	33.70
6	-/169/84	193/6	7	52.93
7	-/169/84	193/6	7	167.53
8	-/169/84	179/6	10	619.53
9	-/169/84	179/6	9	760.49
10	-/208/84	219/6	7	131.63

It can be observed that the linear formulations generally contain more variables and constraints than the convex ones. However, the best linear formulations are still somewhat faster than the convex due to the fact that only one MILP problem need to be solved for linear problems, whereas convex problem formulations require the solution of several MILP subproblems.

4.3.3 The Development of a MINLP Algorithm

Further development of the Extended Cutting Plane (ECP) algorithm has been done with special attention on a new variant of ECP, the alpha-ECP, that is capable of solving pseudo-convex MINLP problems. In a closely related project, an implementation to ECP including a computer interface for a Unix-environment has been built by Mr. Hans Skrifvars. Another MS-Windows application has also been developed. A number of tests with the alpha-ECP have been accomplished.

A convergence proof for global convergence for pseudo-convex MINLP problems can be found in Westerlund et al. (1998c). These extensions to the ECP-

algorithm for convex problems have been implemented and tested on certain examples found in the literature as well as on some pseudo-convex trim loss problems.

The ECP algorithm has also successfully been used for solving convex trim-loss problem formulations.

4.3.4 An Overview of the Tasks

The problems at the paper-converting mill including the trim-loss problem have in more detail been tackled by WalkiWisa Wisapak and Åbo Akademi University. The different issues considering the scheduling problem at the paper converting mill including methodology development are illustrated in the following figure.

In the figure 3 we can see some of the main tasks. This is not an accurate division. Instead, the main purpose is just to give an overview about the relations to the common tasks that have been studied at Åbo Akademi and WISAPAK. One special task, the multi-objective optimization is included in both the scheduling and the trim loss problem, where we e.g. minimize both knife-changes and raw paper usage / trim loss / processing time. This task is of great importance, as will be shown in the study of objectives.

4.3.5 Site-Wide and Operational Considerations

Site-wide and operational considerations comprise an analysis of a process in larger scale and operational issues considering the practical processing matters in functional, energy and environmental aspects.

The task 3 considers the possibility of enlarging production problems to cover more process units or a larger area of the plant. While this task is very case-specific the practical work was incorporated with the case study 2. However, the formulation of the problem is more general and also applicable to other similar problems. The problem considered is a large-scale problem where an expansion to cover more process units may arise significant problems. A lot of work has been done in order to find such a strategy that forms a base of producing good solutions to the problem even in an expanded form.

The specific problem is connected to the final stage of paper making and is to fulfill a set of consumers' demands on paper products. The products should be processed from different raw paper reels roughly by printing, coating, cutting and packing. Finally even the transportation has to be taken into consideration.

Work on investigating the possibilities to include the paper mills together with a paper converting mill has been done. The problems that arise along the transformations (increase of variables and constraints) has been considered in

detail and some new strategies to diminish the original problem have been developed. This has been necessary while the problems considering one part of the whole scheduling problem should be solved in some extent, before an expansion to cover other parts of the process is possible in plant-scale. So far the work has been applied to smaller size problems.

With a new approach there exists potential to expand the original problem without a dramatical expansion of the problem complexity. The basic idea of the strategy is to do the expansion with respect to a small number of variables. Through the strategy a great step towards solving an integrated model can be made. However, there are a lot of possible choices that should be explored. The following general steps are proposed

The procedure is thus iterative and gives as output an expanded model of the original process. For specific problems such as the trim-loss problem the final result cannot be evaluated without performing the following step; the optimization. Therefore, the procedure could be expanded and written as

1. Reduce the original problem by defining tighter bounds and constraints
2. Create a base for expansion by changing some parameters to variables
3. Compare different strategies: which variables should be considered
4. Consider which is a reasonable level of expansion
5. Perform the optimization

A key issue of the methods is that integer programming methods are used instead of some heuristic methods. This approach is very demanding but its results has already shown significant improvements compared to earlier strategies. The proposed methods can find a global optimal solution to the problem which has not been the case for the earlier heuristic or manual methods. However, if the chosen strategy seem to be too demanding for large-scale problems it may be easier to make controlled reductions to the problem by letting the physical constraints determine the reductions of the problems.

4.3.6 Multi-Objective Optimisation

Already in the basic objective, the number of patterns as well as the number of pattern changes are optimized simultaneously. Critical issues are the weight coefficients of the different terms in the objective. Some different objective functions composed with the variables m_j, n_{ij} and y_j have been compared. In the following we try to generate the objective functions for direct minimization of the energy consumption and the waste production to see how well the earlier used objective functions consider these important matters.

4.3.6.1 Minimization of Energy usage

It is quite straightforward to minimize the energy usage:

$$\min\left\{\left(\sum_{j=1}^{J} P_m \cdot l_j / v_m \cdot m_j + P_m \cdot t_j \cdot y_j\right)\right\}$$

where

P_m	is the machine effect (kW)
l_j	is the length of a cutting pattern (i.e. product paper) (m)
v_m	is the machine speed (m/min)
t_j	is the time for a knife change

Note that the result is obtained in kWmin, so the objective value should be multiplied by a factor of 1/60 in order to get the more common unit kWh.

4.3.6.2 Minimization of Waste Production

To minimize the trim loss, i.e. waste production, is a bit more difficult to do at a general level. The trim loss for a pattern can be expressed as

$$m_j \cdot (B_{\max} - B_j) = m_j \cdot (B_{\max} - \sum_{i=1}^{I} n_{ij} \cdot b_i) = m_j \cdot B_{\max} - m_j \cdot \sum_{i=1}^{I} n_{ij} \cdot b_i$$

where

B_{max}	is the raw paper width
B_j	is the total width of the cutting pattern

Thus, we have two alternative formulations

$$\min\left\{\sum_{j=1}^{J} m_j \cdot (B_{\max} - B_j)\right\}$$

or

$$\min\left\{\sum_{j=1}^{J} m_j \cdot B_{\max} - m_j \cdot \sum_{i=1}^{I} n_{ij} \cdot b_i)\right\}$$

The latter expression is bilinear and cannot therefore be used as an objective function without reformulation. Such expressions have been reformulated but the reformulation gave rise to an increase of the number of variables and constraints and is therefore not encouraged. Only in the linear formulation strategy, where we first generate all possible cutting patterns and thus parameterize the variables n_{ij}, we know the width B_j and do not have to decompose the expression for trim loss. Instead, we can straight use the former expression. It should also be mentioned that because of the irregular quality in

the paper edges a cut of 10 mm from both edges is always done. This means that there is always a trim loss of 20 mm. This trim loss will be considered in the following comparison even if it is constant and independent of the strategy used and normally less than 1%. The loss also encourages the use of wider raw paper reels. Unfortunately, the number of feasible combinations is also increased along the width resulting in a more complicated optimization problem.

An earlier study showed that this type of objective function does not give acceptable results while it tends to suggest a great overproduction and does not consider the production time at all. Therefore, a supplement is needed to limit the total number of cutting patterns, m_j. This is done e.g. by adding a +10 term into the parenthesis in the objective function.

$$\min\left\{\sum_{j=1}^{J} m_j \cdot (10 + B_{\max} - B_j)\right\}$$

4.3.6.3 Minimization of Production Time

The energy minimization function can be modified to minimize the total production time.

$$\min\left\{\left(\sum_{j=1}^{J} l_j / v_m \cdot m_j + t_j \cdot y_j\right)\right\}$$

This expression assumes that only one type of a raw paper reel is used because a change of the raw paper width is very time consuming and should be avoided. In the objective above the total time is given in minutes. Moreover, time for setting up the machinery is required. Since that time is almost constant and very difficult to evaluate we leave it unconsidered.

4.3.6.4 A Comparison

In this section some objectives are compared. The simplest objective just minimizes the total number of cutting patterns

$$\sum_{j=1}^{J} m_j$$

where J is the number of different available cutting patterns. If we generate all the possible patterns in advance then this number is equal to the number of possible combinations that satisfy the width and knife constraints (2-4). If the change of the cutting pattern is included the objective changes to the objective of the basic formulation

$$\sum_{j=1}^{J} c_j \cdot m_j + C_j \cdot y_j$$

where C_j and c_j are relative costs for the cutting pattern and the change of cutting pattern. The usage of a binary variable y_j is most recommendable because of the relatively high costs for a change of cutting patterns.

Since the solution performance is not as interesting as the result, a two-step technique is used where all feasible cutting patterns have been determined in advance. Thus, the variables n_{ij} are parameterized and the only variables in the problem are m_j and y_j.

4.3.6.5 The objective functions

From the previous comparison 3 objective functions are compared with the objectives that minimize the energy use (1), waste production (2) and production time (3).

1. $\sum_{j=1}^{J} P_m \cdot l_j / v_m \cdot m_j + P_m \cdot t_j \cdot y_j$
2. $\sum_{j=1}^{J} m_j \cdot (10 + B_{\max} - B_j$
3. $\sum_{j=1}^{J} l_j / v_m \cdot m_j + t_j \cdot y_j$
4. $\sum_{j=1}^{J} m_j \cdot (B_{\max} - f \cdot B_j) + c_j \cdot y_j$
5. $\sum_{j=1}^{J} (B_{\max} / B_j) \cdot m_j + c_j \cdot y_j$
6. $\sum_{j=1}^{J} c_j \cdot m_j + C_j \cdot y_j$

Objective function 4 minimizes the number of knife changes and the waste. The overproduction is also considered. Here we use a factor f = 0.8. Function 5 minimizes both the number of different patterns and the total number of patterns weighted by the width of a pattern. Finally, in the function 6, both the number of patterns and knife changes are minimized with manually determined weights (here: C_j = 1.0 and c_j = 0.1).

4.3.6.6 Example 1

In the following comparison a small and a large order is used to give an overview of the practical daily situations. In the first comparison the following large-size order of 98.74 tons is used:

Product width (mm)	Numbers ordered
350	10
450	28
550	48
650	28
700	40
740	30
800	21
840	22
910	8
960	8
1010	9
1060	8

The results of the optimizations are presented in table 3.

Type	Solution	Time (CPU-s)	Nodes	Iterations	Spill (mm/%)	No. of cuts
1	16800	5190.9	241447	1185195	1540/0.853%	86/9
2	1670	0.03	9	43	640/0.354%	103/10
3	2240	3419.52	172491	909561	1540/0.853%	86/10
4	18943.1	0.55	28	179	980/0.548%	86/13
5	87.379	45.22	1740	6187	990/0.554%	86/10
6	86.9	1509.55	48809	302015	1540/0.853%	86/9

Table 3. The result of the first comparison with the width 2100-2000 mm

The comparison shows that selecting the right objective function is of great importance. Some of the objectives turn out to be unfit for use due to the huge over production, long optimization time or a big waste production. A large number of knife changes prolongs the production time leading to an increased energy demand. The trim loss is often burned to circulate some of the energy back to the process. In the following table we assume a raw paper length of 6500 m and a machine speed of 260 m/min. The energy consumption of a coating machine/slitter is approximated to be 450 kW. The area weight of the coated paper is approximately 0.135 kg/m^2. The time needed for a knife change depends highly on the pattern sequence. In order to simplify the calculations we use here an average of 10 minutes/change.

Type	Production time (min)	Energy Consumption (kWh)	Waste to be burned (kg)	Overproduction (reels)
1	2240	16800	1351.4 (+1509.3)	1
2	2675	20063	561.4 (+1807.7)	49
3	2250	16875	1351.4 (+1509.3)	1
4	2280	17100	860.0 (+1509.3)	1
5	2250	16875	868.7 (+1509.3)	2
6	2240	16800	1351.4 (+1509.3)	1

Table 4. The practical implementation of the optimization results

4.3.6.7 Example 2

In the following, a comparison is made on a mid-size order of 40.46 tons.

Product width (mm)	Numbers ordered
550	8
630	11
685	15
720	5
760	8
810	12
850	6

The results of the optimizations are presented in the following tables

Type	Solution	Time (CPU-s)	Nodes	Iterations	Spill (mm/%)	No. of cuts
1	2925.0	4068.65	76135	672770	945/1.99%	14/4
2	275.0	0.02	32	51	95/0.20%	18/6
3	390	3618.02	63645	586589	945/1.99%	14/4
4	9836.7	19.54	1739	3911	395/0.83%	14/6
5	14.613	573.89	19009	110611	395/0.83%	14/5
6	14.4	3998.72	67893	652290	810/1.7%	14/4

Table 5. The result of the second comparison with the width 3400-3200 mm

In the following table we have used the same parameters as before.

Type	Production time (min)	Energy Consumption (kWh)	Waste to be burned (kg)	Overproduction (reels)
1	390	2925	829.2 (+245.7)	1
2	510	3375	83.4 (+315.9)	28
3	390	2925	829.2 (+245.7)	1
4	410	3075	346.6 (+245.7)	2
5	400	3000	346.6 (+245.7)	2
6	390	2925	710.77 (+245.7)	1

Table 6. The practical implementation of the optimization results

4.3.7 Conclusions

This study supports the results of a number of comparisons where a set of different objectives were considered. When the trim loss is minimized without considering other tasks, the over production becomes a problem. Even if we added a term to consider the total number of patterns, the result was still not applicable. This comparison indicates that attention should be paid also on environmental aspects when formulating the objective function. As a result we can say that the objectives 4 and 5 give the best overall results. Furthermore, there is a clear connection between the production time and energy

consumption. A very interesting property of the objective comparisons that was discovered was the trade-off between different objectives, which makes the problem a very interesting multiobjective problem.

Nomenclature for this section

B_{max} The maximum possible width of a pattern (≈ the raw paper width)
B_j Width of a cutting pattern
m_j Number of times the cutting pattern *j* is used
y_j A binary variable to determine if pattern *j* is used
c_j The cost of a knife change of pattern *j*
C_j The cost of the raw paper for pattern *j*
P_m Energy consumption of a machine (kW)
l_j Length of a cutting pattern/product reel
v_m Speed of a coating machine/slitter
t_j Time for a knife change
f A factor that determines the value of over-production

4.4 Task [T4]: Multi-Objective Optimisation

The objective of this task is to establish a methodology and rigorous algorithmic techniques to solve the integrated design problem that involves more than one, usually conflicting objectives, such as cost, minimisation of energy requirements, environmental impact etc. Within a multi-objective decision framework, the best compromise solution of the design problem depends on the relative importance of the different objectives to the decision maker. It belongs, however, to a set of *non-inferior* solutions, where one objective can only improve at the expense of other objectives.

Nomenclature for this section

I parameter increment
P parametric problem
$\underline{P}$ problem relaxation
$\overline{P}$ problem overestimator
p parameter
p^{lo} lower bound of parameter p
p^{up} upper bound of parameter p
p_k parameter value at k-iteration
$p^{lo}g$ global lower bound of parameter p
$p^{up}{}_g$ global upper bound of parameter p
$p^{lo}{}_{cur}$ current lower bound of parameter p
$p^{up}{}_{cur}$ current upper bound of parameter p
$p^{lo}{}_{klo}$ lower bound of parametric interval at k-iteration, where problem relaxation is feasible
$p^{up}{}_{klo}$ upper bound of parametric interval at k-iteration, where problem relaxation is feasible
$p^{lo}{}_{kup}$ lower bound of parametric interval at k-iteration,

where problem overestimator is feasible

p^{up}_{kup} upper bound of parametric interval at k-iteration where problem overestimator is feasible

y binary variable (or variable vector)

y_0 initial binary vector

$y_{k,I}$ binary vector in i-parameter inerval and k-iteration

z_k value of objective variable corresponding to p_k

z^* optimal solution

$z^{up}_{k,i}$ upper bound of objective variable z in i-interval and k-iteration

$z^{lo}_{k,i}$ lower bound of objective variable z in i-interval and k-iteration

4.4.1 Extended Cutting Plane Algorithm

The development of the Extended Cutting Plane (ECP) algorithm is been done and special attention is paid on a new variant of ECP, the alpha-ECP, that is capable of solving a pseudo-convex mixed integer non-linear programming (MINLP) problem. In a closely related project, an implementation to ECP including a computer interface is under work. Extensive tests with the alpha-ECP has been carried out and work will continue on testing and developing this strategy.

A convergence proof for global convergence for pseudo-convex MINLP problems has already been made. These extensions to the ECP-algorithm for convex problems have been implemented and tested on certain examples found in the literature as well as the optimisation problems encountered in the paper mill trim-loss Case Study. This topic of study has been fully dealt within the Task [T3] report section.

4.4.2 Decomposition based Multi-Objective Optimisation

Multiobjective optimization techniques have been explored in CPERI for mixed integer nonlinear problems, focussing on the identification of the noninferior solution sets. Two main cases have been examined:

- Convex design problems (Convex MINLPs)
- Nonconvex design problems (Nonconvex MINLPs)

Multi-objective optimization for convex MINLPs

The extended algorithm for the identification of non-inferior solution of convex, multi-objective MINLP problems is illustrated in Figure 1.

The main features of the algorithm are:

⇒ The initial multiobjective MINLP problem is formulated as a multi-parametric MINLP problem, where the parametric regions of interest are identified solving scalar MINLP problems (for each objective separately). The

non-inferior solution set is constructed then in an iterative manner, as the parametric solution of the multi-parametric MINLP problem.

⇒ Parametric upper bounds to the optimal solution are identified in each iteration, with the solution of parametric NLP subproblems that result by fixing the integer (binary) variables of the original problem.

⇒ A parametric lower bound is updated in each iteration via the solution of a parametric MILP Master problem, that involves only the binary variables of the initial problem and Lagrangian cut-constraints based on the parametric continuous optimization steps.

Convergence properties and computational requirements of the algorithm have been studied with the solution of numerical examples from the literature. It results that the proposed algorithm performs efficiently for two-objective problems, compared to established parametric optimization techniques. For more that two-objective MINLP problems, the computational requirements increase dramatically, as the solution of multi-parametric NLP and MILP problems is required; still, compared to current techniques for parametric optimization, less NLP and MILP subproblems are required to be solved.

Algorithmic developments and numerical examples are presented in detail in the final IDEES report on Multiobjective Optimization techniques.

Multi-objective optimization for non-convex MINLPs

Two algorithms have been developed for the solution of nonconvex parametric MINLP problems and the identification of the noninferior solutions of multiobjective MINLP problems.

a. The first one is based on the ε-constraint method (Clark and Westerberg, 1983). The main ideas of the algorithm are:

⇒ The initial multi-objective problem is formulated as a multi-parametric MINLP problem, where the secondary problem objectives are treated as parametric constraints.

⇒ The parameter space of interest is discretized and a scalar MINLP problem is solved at each parameter point.

When global optimality is not of interest, local optimization methods can be applied for the solution of the nonconvex MINLP problems. The generalized Benders decomposition methods (Geoffrion, 1972) has been employed in this project for the local optimization of the scalar MINLP problems. Alternatively, the αBB-gMIN method of Adjiman *et al.* (1997) has been explored for the solution of each scalar MINLP of the ε-constraint method, in

order to guarantee global optimality. As expected, computational effort is increased significantly when global optimality is required.

⇒ The optimal parametric solution is approximated by piece-wise linear functions of the parameters, within the regions that are defined by the parameter points where the initial problem is solved. The accuracy of the approximation is improved employing a finer discretization of the parameter space and increasing accordingly the computational requirements of the method.

For the scalar parametric case (two objectives) the method is illustrated in Figure 2. Details and performance of the algorithm are discussed in the final IDEES report on Multiobjective Optimization techniques.

b. For scalar parametric MINLP problems (or equivalently, MINLP problems with two objectives) an alternative algorithm is developed for the derivation of the global optimal parametric solution via an upper- and lower- bounding procedure. The main idea of the algorithm is the construction of *valid* parametric upper and lower bounds to the global optimal parametric solution in an iterative manner and through a spatial branch and bound search of the variable space. In particular:

⇒ The parametric upper bound is found considering a *convex overestimator* of the initial problem. The line segment that is defined by solving the convex overestimator at two parametric points is a valid upper bound to the optimal solution of the overestimator and, thus, to the optimal solution of the actual problem.

⇒ The parametric lower bound is found solving a *convex relaxation* of the initial problem at a parametric point and considering the tangent line (linear parametric function) to that point. Due to convexity, that is a valid lower bound to the convex relaxation and, thus, to the initial problem.

⇒ The parametric upper and lower bounds are updated in each iteration, where the variable space is partitioned into subspaces (nodes of the spatial branch and bound), resulting, thus in tighter bounds. The upper and lower bounds converge to the optimal solution in a finite number of iterations within a ε-tolerance.

The algorithm is illustrated in Figure 3. Computational requirements and applicability of the algorithm are discussed in detail in the final IDEES report on Multiobjective Optimization techniques.

Conclusions

Parametric optimization algorithms have been developed within the IDEES project for the identification of the noninferior solutions of multiobjective design/synthesis problems, which involve discrete and continuous decisions and

are formulated as multiobjective MINLP problems. For the particular case of convex MINLP problems the developed optimization method has proved computationally efficient compared to established methods. Naturally, as the number of objectives increases, the required computations increase accordingly; however, not more than three objectives are common in design problems (e.g. cost, energy, environmental impact). For general nonconvex MINLP problems, it has been found that in order to guarantee global optimality of the parametric solution the computational requirements increase dramatically. Nevertheless, the suggested algorithms are still the only available techniques to guarantee global optimality in multiobjective problems.

4.5 Task [T5]: Computer-Aided Design Tools

The Computer-Aided Design tool-kits are focusing on the application areas characterised by the specific industrial processes studied. The two resulting prototype tool-kits have a broad range of generic applications. At the heart of both developments is a capability for multi-objective mixed-integer non-linear optimisation. It is believed that the software developed in IDEES is the first successful industrial application of such optimisation and the first that has been made sufficiently generic for wide scale application. The following two sections cover these two applications, trim loss minimisation and pre-heat train optimisation.

4.5.1 Introduction

The underlying research has developed the process models and integrated them with mixed integer optimisation routines. It has demonstrated the potential benefits of applying these optimisation strategies in practice. The objective of Work Package 5 (CAD Tools) is to encapsulate the optimisation within a readily accessible User Interface that enables the tools to be used routinely in an industrial context. In this way, the benefits of the research are made available to European Industry.

In this chapter, we give a brief description of the Wisatrim package which encapsulates the research at Abo Akademi applied to the paper finishing industry. We also give a description of the IDEES-NET package that attempts to encapsulate the research at Imperial College and CPERI in a way usable by Statoil.

IDEES-NET cannot be routinely applied until the Statoil revised pre-heat train comes on line in the fourth quarter of this year. Until that time, we can only judge that it is likely to be useful. It shows potential energy savings of up to 5% for the design feedstock and operating conditions. It is likely that, later on the plant life, different feedstocks have to be used, and different product mixes will

be required. At that stage, the ability to re-optimise operating conditions within a few minutes may pay greater financial and environmental dividends.

4.5.2 Trim Loss: The WISATRIM Program

The Wisatrim package directly employs the software developed at Abo Akademi. Briefly the optimisation procedures developed at Abo Akademi have been provided with a user- friendly Graphical User Interface by Wisapak, who have paid all the necessary costs for software licences, and have developed the User Interface using their own resources.

Wisatrim is already routinely used, and will be used more widely within Wisapak world-wide. It has already demonstrated waste reductions of up to 30%, along with increased plant throughput.

4.5.3 Preheat optimisation: The IDEES-NET Program

This program takes the basic optimisation models as developed, and published, by CPERI and recodes them in a new package. The whole package runs on a PC operating under Windows NT or Windows 95. In this way, it is easily integrated with other packages used by Statoil. In this section, we describe each of the main parts of the program in turn, the optimiser, the mathematical models, and the User Interface.

4.5.3.1 Optimisation

The optimisation framework employed by CPERI is the GAMS software. GAMS is cheaply available to academic institutions, but is very expensive for industrial partners. Furthermore, it is not easy to provide it with a user interface geared to non-specialist end users. At the same time, it has not proven to be very robust. CPERI have needed to use great skill to generate starting estimates from which the optimiser will find a good solution.

Statoil require a cheap, reliable program with a user interface which works smoothly with tools that they are already using. For this reason, we have sought an alternative optimiser. After evaluating a number of options that might have been available to us, we decided to employ Filter SQP. Filter SQP has been developed at Dundee University as part of another collaborative research programme involving QuantiSci. (The ECOSSE research consortium). Tests have shown that Filter SQP is between 1 and 2 orders of magnitude faster than its immediate competitors. It also appears to be more robust. Certainly it has solved pre-heat train optimisations from starting estimates at which other codes failed.

The features of Filter SQP are that it is a successive Quadratic Programming optimiser using Branch and Bound for its integer variables. The SQP uses an

active set method of handling constraints, rather than the more popular barrier function methods. It has an interface that enables it to read problems defined in the standard SIF input format. The SIF format is a (not very elegant) method of defining non-linear constrained optimisation problems as a set of equations and inequalities. The SIF format enables both first and second derivative equations to be defined. Filter SQP demands that both first and second derivatives are defined. This requirement has placed some limitations on the complexity of the equations that it is practicable to employ. The consequences of these limitations are discussed in Section 3.2 (the mathematical models). SIF does not define a standard for specifying integer constraints. Filter SQP therefore handles integer variables in a second file adapted from the SIF standard.
In practice, it seems likely that the immediate requirements placed by Statoil can be met without using integer variables. (It is well known that some binary variable integer problems can be handled without recourse to specifically integer formulations. In these problems, the binary variables all finish against constraints, thus taking the values 0 or 1). We have, however, the option of introducing integer variables explicitly if necessary.

4.5.3.2 The mathematical models

All the models are adapted from the models developed by CPERI. In summary these are:

- Physical Properties. We used a linear heat capacity versus temperature relationship identical to that developed by CPERI. Indeed, we used the same coefficients derived by them.
- De-salter. We specify an acceptable operating temperature range. The range can be set either as upper and lower bounds, or as an equality.
- Distillation heat loads. The off-take temperature of each side stream from a distillation column is specified. The total heat abstraction for each returned stream is specified. The flow rate of each returned stream can be optimised within pre-set ranges.
- Stream splitters. The splits can be optimised, with bounds set on each of the outlet flow rates. The bounds can be equalities, or upper and lower bounds.
- Heat exchangers. A slightly different log-mean temperature approximation is used than that employed by CPERI. Thus we use:

$$T_m^3 = DT_1 \omega DT_2 \omega \frac{1}{2}(DT_1 + DT_2)$$

where T_m is the mean temperature difference, and DT_1 and DT_2 are the temperature differences at each end.

The advantages of the above expression are:

i) It is as good an approximation when DT_1 and DT_2 are similar
ii) It correctly goes to zero whenever DT_1 or DT_2 go to zero. This feature is important because it ensures that the heat transfer rate goes to zero if either of the temperature differences go to zero. In this way, we avoid temperature

cross-over which is both physically impossible, and gives rise to nasty optimisation problems

iii) It is smoothly continuous through zero. Thus, even for physically unreasonable values, it avoids local discontinuities which can cause optimisers to fail

iv) It is easily twice differentiable (which is important for Filter SQP).

We have taken care of the mathematical properties to ensure a smooth optimisation that is relatively insensitive to starting estimates. It may be considered that this concern for numerical characteristics has compromised the accuracy of the models in representing the actual physical performance. This is not the case. The log-mean temperature itself is simple approximation that is only valid if U is everywhere the same throughout the exchanger, and if all values of specific heat are constants. If U varies linearly with temperature the correct log mean is to take the log-mean of ($U_1 \omega DT_1$) and ($U_2 \omega DT_2$). This value differs more from the mean U times the mean DT than our approximation. Similarly, if Cp varies with temperature, the log mean does not predict the correct heat transfer rate. We have derived more accurate expressions. However, in practice, heat transfer coefficients are computed from measured plant data. Providing they are fitted using the same heat transfer model as in the optimisation, the calculate heat transfer rates at nominal conditions will be computed correctly. We are then only concerned at how good the models are when conditions move away from nominal. For this purpose, all the models seem to be about equally good. Indeed, including heat transfer effectiveness then only makes the predictions better by 1% to 2%. The resulting predicted optimal operating conditions are then hardly changed. For this reason, and to give a robust optimisation, we have taken heat transfer effectiveness as fixed for this first release. We have derived a simpler smooth form for the prediction of effectiveness if it is required for a later release.

Pressure drop constraints through the exchangers are included by setting maximum permissible flow rates for each main process stream.

- Steam-raising water coolers. Instead of fixed heat duty exchangers, we have modelled these as conventional exchangers. We have locally optimised cooling water flow rate to maximise steam production for any oil inlet conditions. This local optimisation is valid on the basis that it can be increased without adjusting conditions elsewhere. Any condition in which steam production is not locally optimised is thus not a global optimum. This approach gives a more realistic overall process model without complicating the optimisation significantly. Indeed, by abandoning the fixed heat load assumption, we make it less likely that physically impossible conditions will arise during the optimisation. This, in turn, makes the optimisation simpler and more robust.

- Air coolers. These were previously modelled as fixed outlet temperature coolers. This model was clearly physically unrealistic. It would even allow outlet temperatures below ambient. Furthermore, even with very low outlet

temperature differences, it could predict very large heat transfer rates. The optimisation was then left with no penalty for delivering high flow rates of hot oil to the coolers. In consultation with Statoil, we have employed a rather more realistic model. Thus, for a pre-defined outlet temperature difference, we take a maximum heat load on the exchanger. This heat load cannot be exceeded. We then set a target outlet temperature. If the required heat load to meet this temperature is less than the maximum heat load, we assume that the target temperature can be met. If it cannot be met, there are two possible modes of operation. In the first mode, we allow the outlet temperature to go above the outlet target. The user can immediately spot such conditions and set a constraint that reduces the permissible flow rate through the cooler or reduces the inlet temperature to the cooler. In the second mode, we set the heat load as a hard constraint, but put a much higher penalty if the target outlet temperature cannot be met. In principle, the relevant oil flow rates will then be driven down. We have decided to employ the first mode of operation. The reason is, that the second mode would enable a user to set conditions for which the constraints would be impossible, or virtually impossible to meet. The optimiser might then fail with no obvious recourse open to the user.

- Mixers. We retain the earlier simple isenthalpic mixer models.

4.5.3.3 Graphical User Interface

We have adapted the standard PC spreadsheet Excel as a User Interface. The benefits of this approach are:

i) It is an interface that Statoil (and most other potential users) are fully familiar with
ii) It enables Users to cut and paste inputs from other Windows programs. Similarly, it enables results to be cut and paste to other tools for post-processing
iii) It enables the standard Excel facilities to be used for data preparation and post-processing
iv) It provides graphing tools etc. without any special programming effort.
v)

The GUI enables upper and lower bounds to be set for all appropriate variables. It has built in checks that values supplied are reasonable (typically checks that upper bounds are greater than lower bounds and that lower bounds are greater than zero). It also checks for reasonable orders of magnitude. It provides default values and starting estimates from which reliable convergence should be achieved.

4.6 Task [T6], Case Study 1: Crude Oil Preheat System

The integrated framework for the synthesis of energy efficient processes, that has been developed within the IDEES project, has been applied to the crude preheat section of Statoil's refinery in Kalundborg.

4.7 Task [T6], Case Study 3: Methanol Production

4.7.1 Problem formulation

In an industrial process flowsheet, a mixture coming from methanol production is separated into 99.999% pure methanol (3125 kmol/hr) and 91% pure carbon dioxide (9.399 kmol/hr). The multicomponent mixture are listed in Table 1, and the product specifications are 99.999% purity and 99% recovery of methanol, and 91 % pure carbon dioxide.

Table 1: Components in the methanol example and its composition

Compounds	*Composition (kmoles/hr)*	*Composition (mole %)*
Carbon dioxide (CO_2)	35.7	0.905
Acetone (CH_3-CO-CH_3)	0.052	0.0013
Methanol (MeOH)	3155.35	80.0
Ethanol (EtOH)	1.45	0.0368
Water (H_2O)	750	19.0
Butanol (BuOH)	1.079	0.027

4.7.2 Feasible flowsheets

Employing the developed methodology for synthesis and design of separation systems (Jaksland C., 1996, Ph.D. Thesis) a physically feasible flowsheet for separation of a mixture from methanol production has been generated (see Figure 1). After the reactor, the mixture consists of carbon dioxide, methanol, ethanol, water and butanol. Based on large differences in volatility (vapour pressure) between carbon dioxide and acetone, flash operation is identified. Based on analysis of the influence of P, T and $\underline{x}$ on the properties and phase diagrams conditions of operation are 1 atm and 315K. The mixture splits into a vapour product (2) and a liquid product (3). Based on large differences in water solubility absorption is identified for separation of carbon dioxide from the polar mixture components. The solvent is water. This results in a stream rich in carbon dioxide with a small amount of water (8) and one stream with methanol, water, butanol, acetone and ethanol (7). Stream (8) is purified employing adsorption, where a polar adsorbent may be employed for dehydrating the carbon dioxide to 99.9% purity. Stream (7) is mixed with stream (3). For stream (9), distillation is identified between acetone (and any lighter by-products) and methanol. Acetone forms a pressure sensitive, low boiling azeotrope with water, which vanishes at pressures 0.6-0.7 atm. This results in a carbon dioxide rich product, polluted with a small fraction of methanol (11). The heavier alcohols and the water leaves as bottom product (10). Finally, based on large differences

in volatilities, distillation is identified for separation of 99.98% pure methanol, 3142 kmoles/hr (12) from a mixture of water and alcohols (13). This separation is carried out at P=1 atm, and top and bottom temperatures are estimated from the boiling points of pure methanol (337K) and water (373K) respectively. The adsorbent unit could not be simulated, since we at present do not have computational tools for adsorption processes.

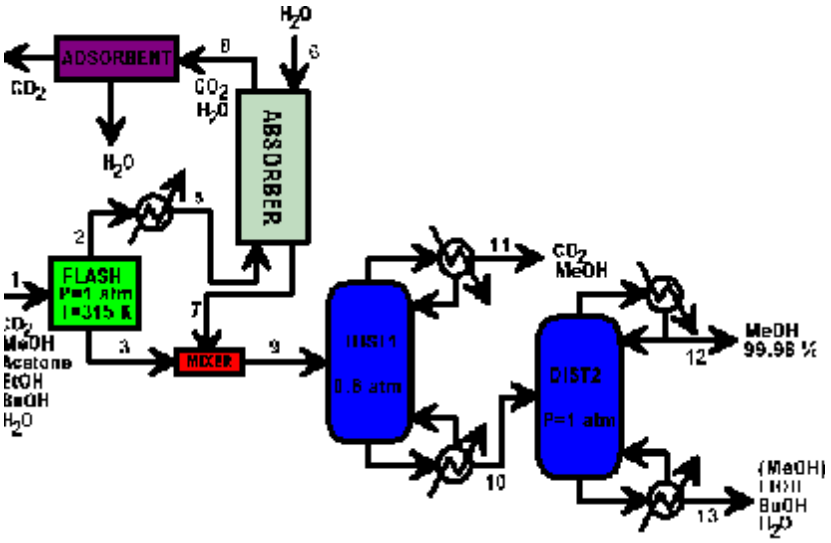


Figure 1. Flowsheet alternative 1

Energy Cost:
For this flowsheet the total energy consumption is 1.2815×10^6 MJ/h.

In Figure 2, a flowsheet alternative is illustrated which has been verified with process simulation as physically feasible (all units except the pervaporation unit). As illustrated, the absorber may be substituted with a flash. The methanol production is 3122 kmoles/hr of 99.99% purity.

Energy Cost:
For this flowsheet the total energy consumption is 1.2691×10^6 MJ/h.

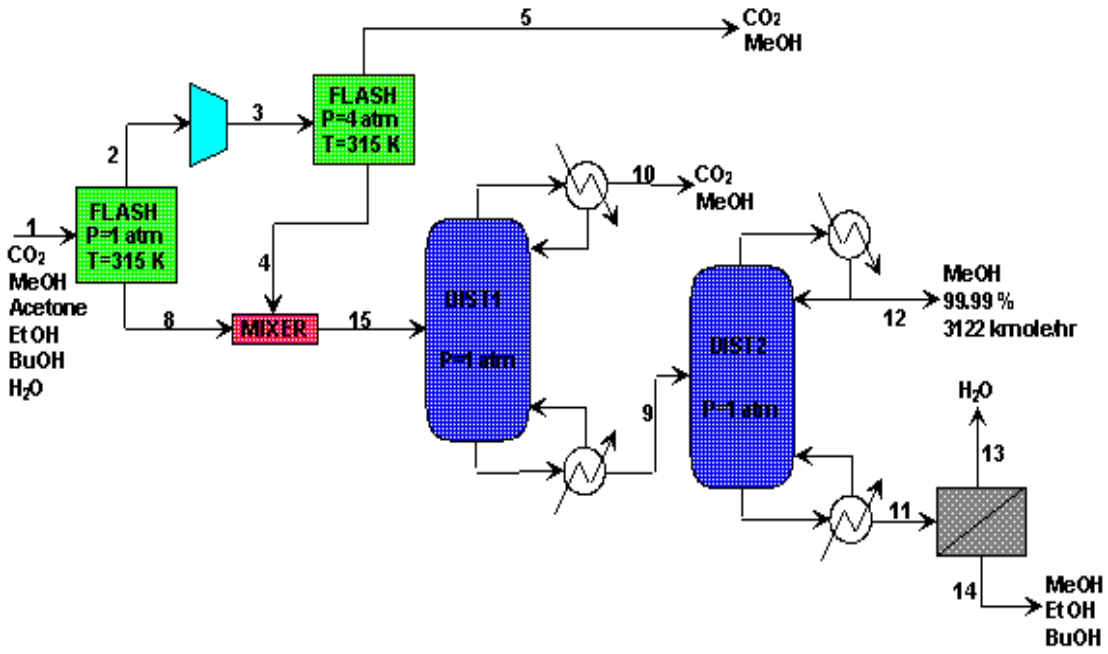


Figure 2. Flowsheet alternative 2

Flowsheet alternatives 3, 4 and 5 are shown in the next Figures 3, 4, and 5 respectively. All of them have been verified with process simulation as physically feasible.

Figure 3: The methanol production is 3135.11 kmoles/hr of 99.98% purity.
Energy Cost: For this flowsheet the total energy consumption is 1.9159×10^6 MJ/h.

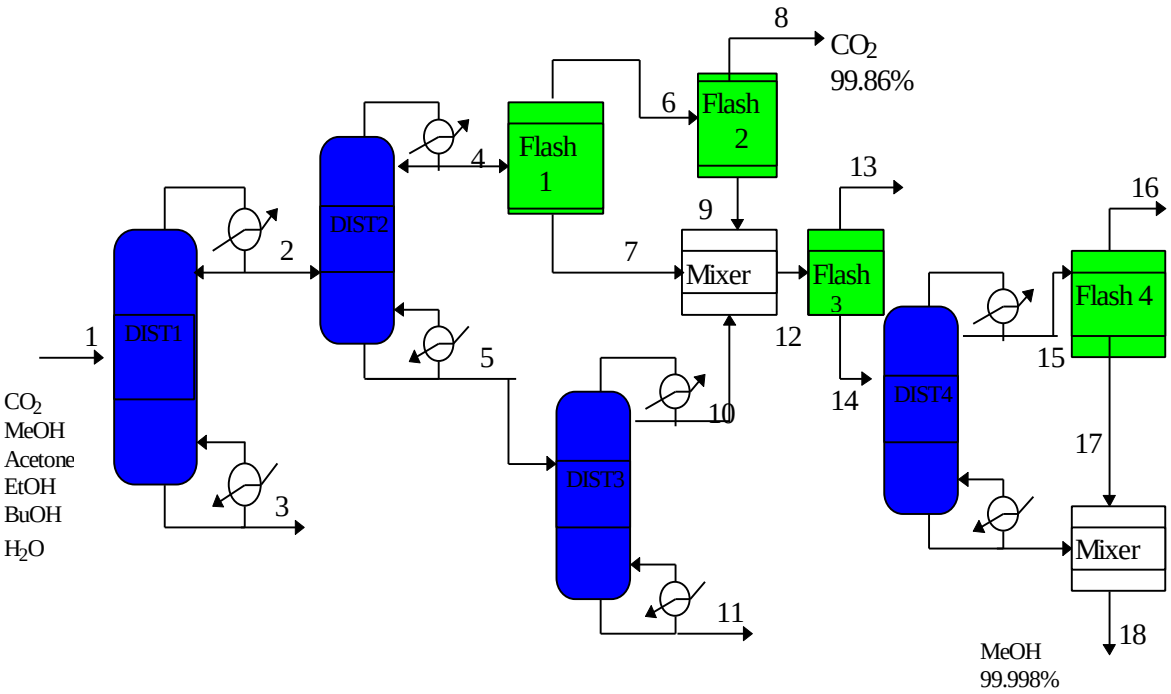


Figure 3. Flowsheet alternative 3

Figure 4: The methanol production is 3137.94 kmoles/hr of 99.95% purity. Energy Cost: For this flowsheet the total energy consumption is 0.52999×10^6 MJ/h.

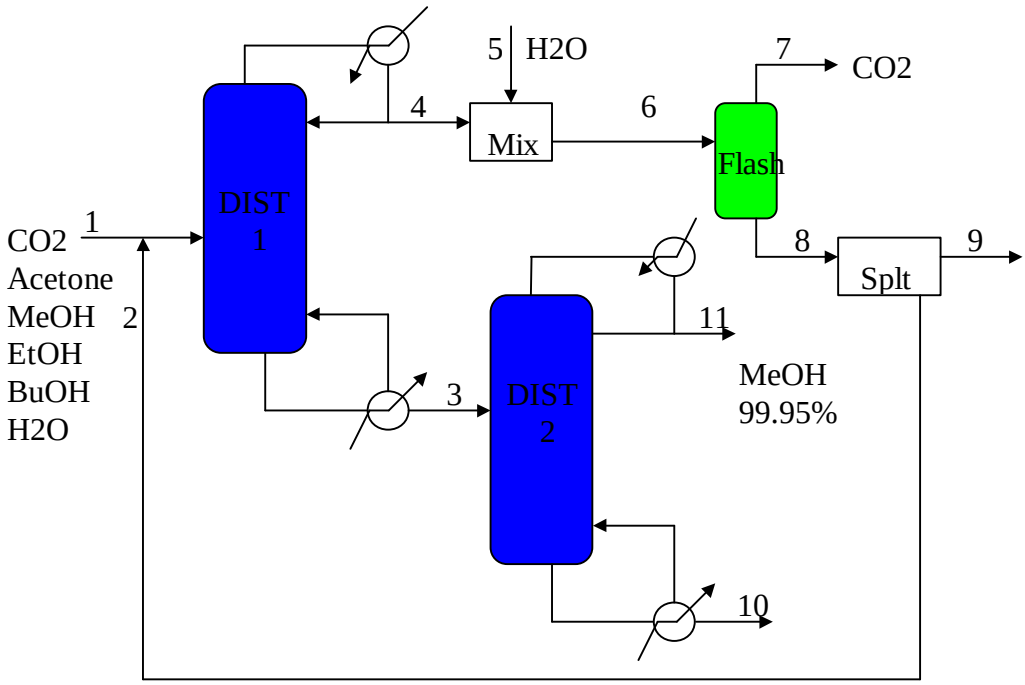


Figure 4. Flowsheet alternative 4

Figure 5: The methanol production is 3126.26 kmoles/hr of 99.998% purity.
Energy Cost: For this flowsheet the total energy consumption is 0.4728×10^6 MJ/h.

The flowsheet of alternative 5 was developed considering the following points,

- The most important separation are between CO_2-MeOH-H_2O, because they has the biggest concentrations. The feasible technique for this separation is a distillation column.
- The flashes have been found inefficient.
- With the optimisation task of the SEPSIM package, the conditions of operation of the flowsheet was optimised.

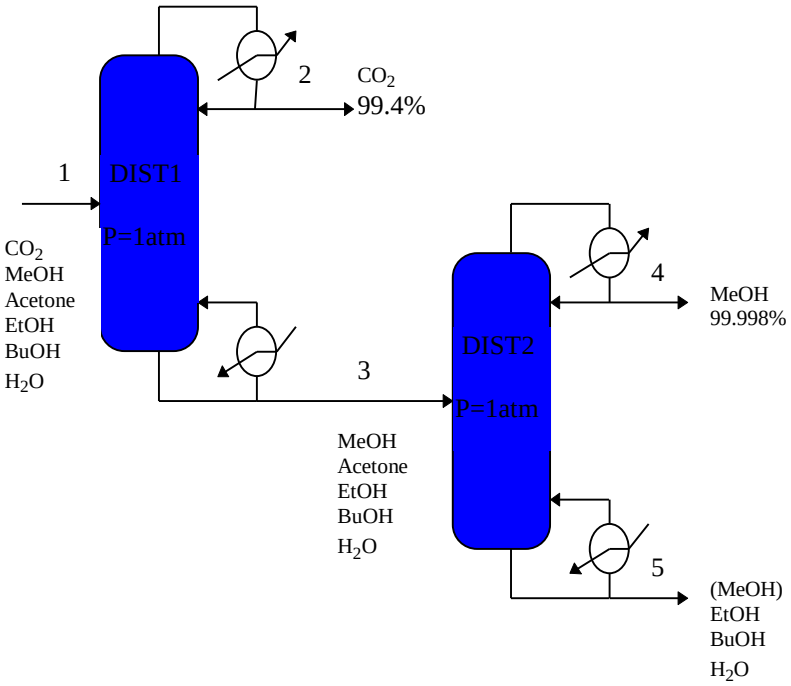


Figure 5. Flowsheet alternative 5

4.7.3 Application of the Mass/Heat Transfer Framework

This section describes the application of the mass/heat transfer framework to the methanol case study, as described below.

Problem Statement

Given
- the multicomponent feed mixture of 3944.071 kmol/h at 1atm, 308K
of component flowrate as given in Table X to be separated

- desired product specification of

$F1_{prod} > 3125$ kmol/h $F2_{prod} > 9.339$ kmol/h

$X1_{MeOH,\ prod} > 0.9999$ $X2_{CO2,\ prod} > 0.91$

- available as heat utilities steam and cooling water
- available as mass utilities water

Synthesise a feasible separation system that is optimal with respect to utility costs (i.e. energy requirements).

Thermodynamics

Accurate description of the vapour-liquid equilibria is necessary to capture the characteristics of the mixture, which features nonidealities. In addition, the presence of carbon dioxide required special consideration.

For enthalpy calculations,

$$H_{vap}(T) = \int_{Tref}^{T} Cp_{pg}\, dT$$

$$H_{liq}(T) = \int_{Tref}^{T} Cp_{pg}\, dT - \Delta H_{evap}$$

$$\Delta H_{evap} = A_i\,(1 - Tr_i)^{B + C\,Tr + D\,Tr2}$$

where the required pure component parameters were obtained from the SEPSIM databank. Note that for carbon dioxide, a constant heat of vapourisation was utilised.

For calculation of the fugacity coefficient, the SRK equation of state with MHV2-UNIFAC model was used to match the thermodynamics used in the analysis and designs carried out in the previous section.

Synthesis Framework

The mass/heat transfer representation framework as applied to the given separation task involves the following features.

Mass/heat transfer module

Within the mass/heat transfer representation, process operations are modelled as sets of mass and heat exchangers between two properly defined streams (Papalexandri and Pistikopoulos, 1996). In this manner, units and structures need not be explicitly pre-postulated but instead investigated as mass and heat exchange possibilities between streams. The building block of this modelling framework is defined as a mass/heat exchange module connected to pure heat exchanger blocks (Figure \ref{fig:module}). Side mixers and splitters are assigned to each mass/heat exchange module and heat exchanger, allowing for all possible interconnections between exchangers (interconnections are assumed

to be of the same phase). The core of the representation, the modelling of mass transfer within the module, will be discussed later.

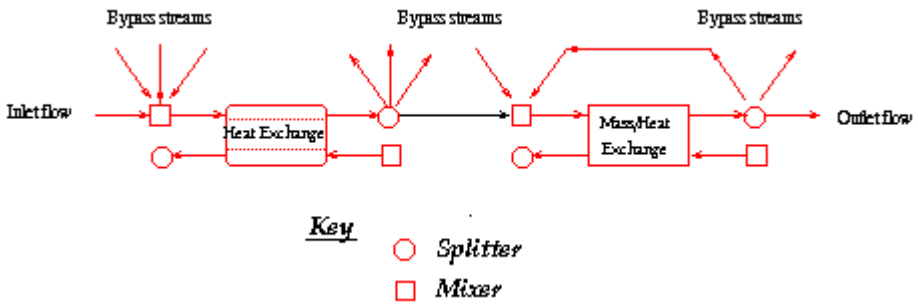


Figure 1 : A mass/heat transfer module

Stream superset

A liquid and a vapour general mixed stream containing all components is considered to account for all possible initial, intermediate and final streams that may exist in the system. This implies that components are miscible in all phases, and therefore we only consider conditions whereby no liquid-liquid separation occurs.

Mass/heat exchange matches

For the separation of homogeneous mixtures, mass transfer can occur between liquid and vapour streams due to volatility differences. Furthermore, multicomponent mixtures exhibit more than one mass exchange patterns. Therefore multiple liquid-vapour stream matches corresponding to multiple mass/heat exchange modules are considered. The number of multiple matches defines the complexity of the superstructure and as the number of matches increases, the detail and quality of the representation improves at the cost of numerical complexity. For numerical purposes, an upper bound is imposed on the number of modules.

Mass Driving Force Constraints

A mass/heat module for separation may represent a part or whole of any separator, such as a single tray or aggregate of trays in a distillation column. Mass transfer takes place between adjacent streams when their corresponding compositions are not at equilibrium. Mathematically, this can be modelled by the following logical conditions;

$$(g_1 \geq 0 \wedge g_2 \geq 0 \Rightarrow g_3 \geq 0) \vee$$
$$(g_1 \leq 0 \wedge g_2 \leq 0 \Rightarrow g_3 \leq 0)$$

where

$g_1 = f_i^{li} x_i^{li} - f_i^{vo} x_i^{vo}$ distance from equilibrium at liquid inlet

$g_2 = f_i^{lo} x_i^{lo} - f_i^{vi} x_i^{vi}$ distance from equilibrium at liquid inlet

$$g_3 = F^{li}x_i^{li} - F^{lo}x_i^{lo} \qquad \text{mass transfer direction}$$

where the superscripts *li,lo,vi,vo* denote the liquid inlet, liquid outlet, vapour inlet and vapour outlet streams respectively, f_i is the fugacity coefficient, F the molar flowrate and x_i the molar composition.

The above logical conditions can be recasted in the following compact mathematical form (Ismail *et al.*, 1997, 1998):

$$\begin{aligned} g_1 g_2 &\geq 0 \\ g_1 g_3 &\geq 0 \end{aligned} \qquad (1)$$

Note that mass transfer direction is not postulated in the expressions in equations (1). Further, the bilinear terms can be recasted in a linear form by the introduction of binary variables to denote the mass transfer direction in the module (Ismail *et al.*, 1998).

Mass/heat exchange network superstructure

In general, a superstructure involving all possible interconnections between the splitters and mixers of the building blocks is defined (Figure 2) and logic is applied to screen out interconnections that cannot exist to result in a reduced superstructure (e.g. recycling of a stream that has just been separated is illogical and not allowed).

Here we utilise the feasible structures generated by DTU (shown earlier) as an additional guideline to formulate a superstructure of alternatives. Part of the superstructure is shown in Figure 3, which encompasses flowsheet alternatives 2,3,4 and 5. A set of at least 6 possible products is allowed for, equating the number of stream components.

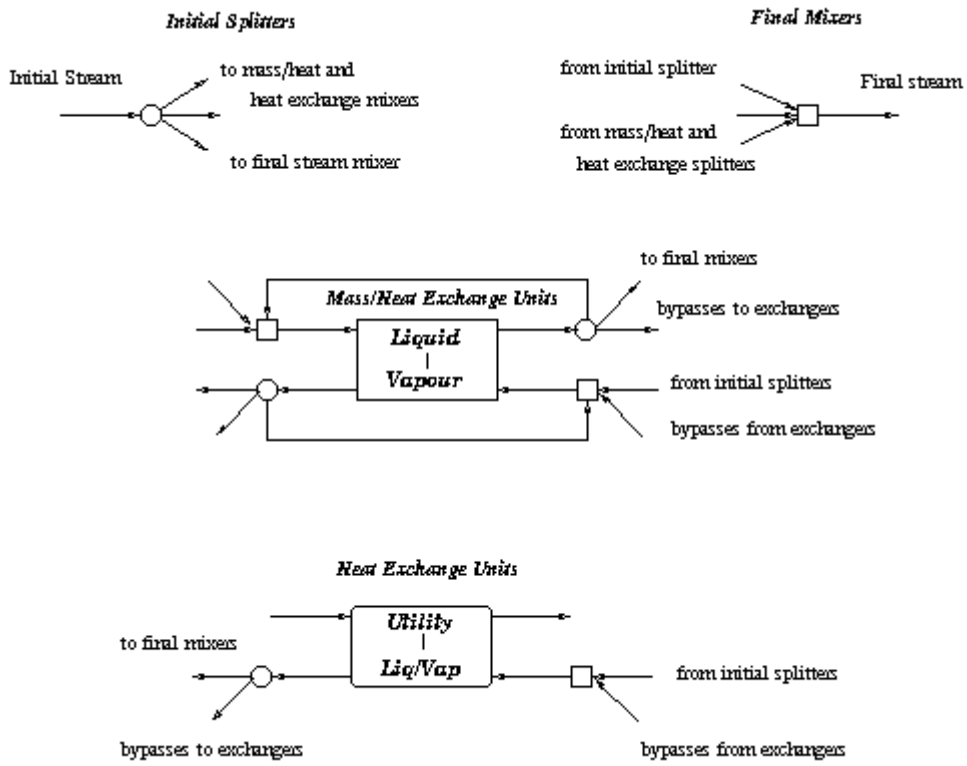


Figure 2 : Superstructure building blocks

Superstructure model

Binary variables are introduced to denote (i) the existence (or not) of each module, (ii) existence (or not) of interconnecting streams between the splitters and mixers and (iii) the mass transfer direction for each component in each module. Note that variables (ii) are not necessary, thus their presence does not increase the combinatorial complexity of the synthesis problem. They are utilised to simplify the solution of the nonlinear part of the superstructure model and to facilitate the introduction of logical constraints to the model. Similarly, variables (iii) are not necessary and its inclusion simplifies the mass transfer driving force constraints.

The mass/heat exchange network superstructure model is formulated as a mixed integer optimisation problem (MINLP), involving the following:

- total mass balances at the splitters, total and component balances at the mixers of the
superstructure.
- component mass balances at the mass/heat exchangers.
- energy balances at the mixers, pure heat and mass/heat exchangers.
- summation of stream molar fractions.
- phase defining constraints for each stream, ensuring that the temperature of liquid streams are at most the mixture boiling point (bubble point), and that of vapour streams are at least the mixture dew point.
- driving force constraints at mass/heat exchangers.

- temperature-based driving force constraints for heat exchange at the inlet and outlet of heat exchange units.
- thermodynamic property calculation of each stream as a function of its temperature, composition and pressure, including enthalpy, and fugacity coefficient calculation. Note that any thermodynamic model and correlation can be incorporated.
- mixed integer constraints to account for the existence of modules and interconnections
- pure integer constraints corresponding to logical conditions or process constraints, reducing combinatorial complexity.
- Objective function consisting of the cost of heat utilities.

The problem is modelled in GAMS Modelling Language (Brooke et al., 1988).

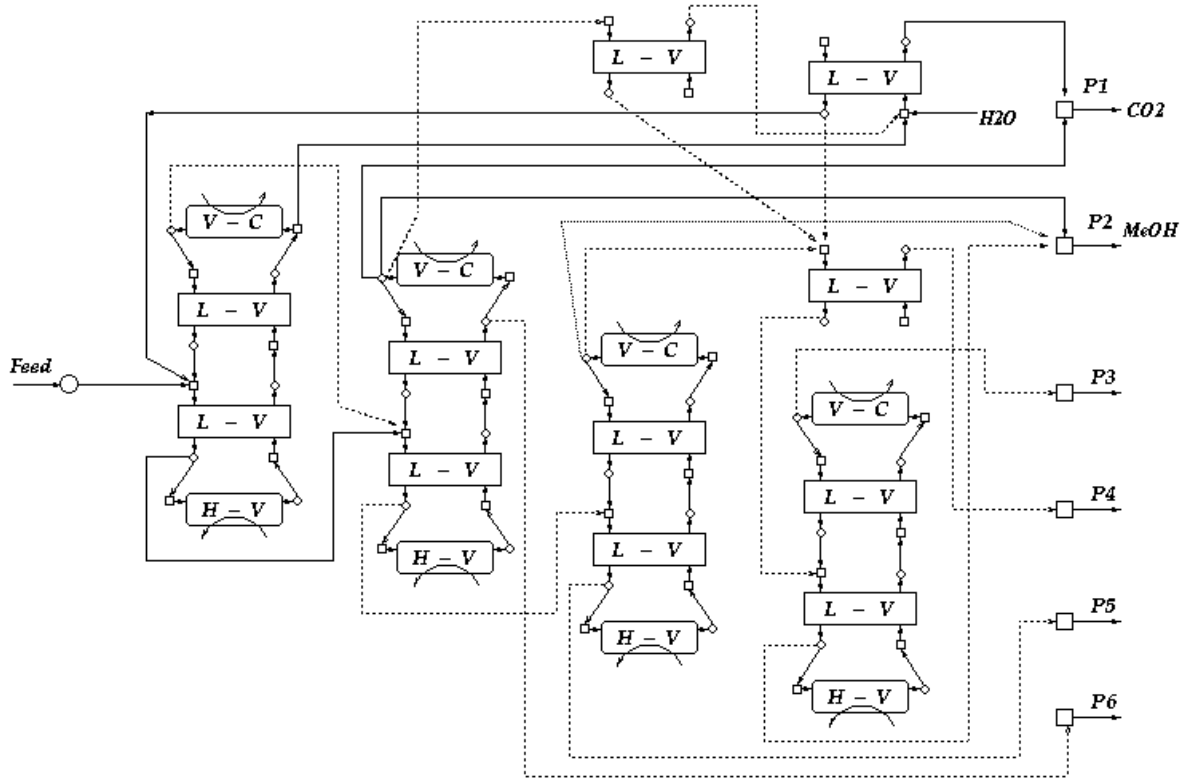


Figure 3 : Mass/heat exchange superstructure

The full MINLP has not been solved to optimality but alternatives can be generated. The result with the lowest utility cost is shown in Figure \ref{fig:opt}, consisting of four mass/heat exchangers and two pure heat exchangers. This configuration is the same as Flowsheet Alternative 5, representing two separator columns. Module *MH1* represents a rectifying section and module *MH2* a stripping section. In both these modules, carbon dioxide and acetone is transferred from the liquid to the vapour stream. The remaining components are transferred from the vapour to the liquid stream, excepting methanol which is also transferred to the vapour stream in *MH2*. The streams of modules *MH3* and *MH4* consist mainly of methanol, with traces of

ethanol, water and butanol. In these modules, the methanol is transferred to the vapour stream, and the other components to the liquid stream.

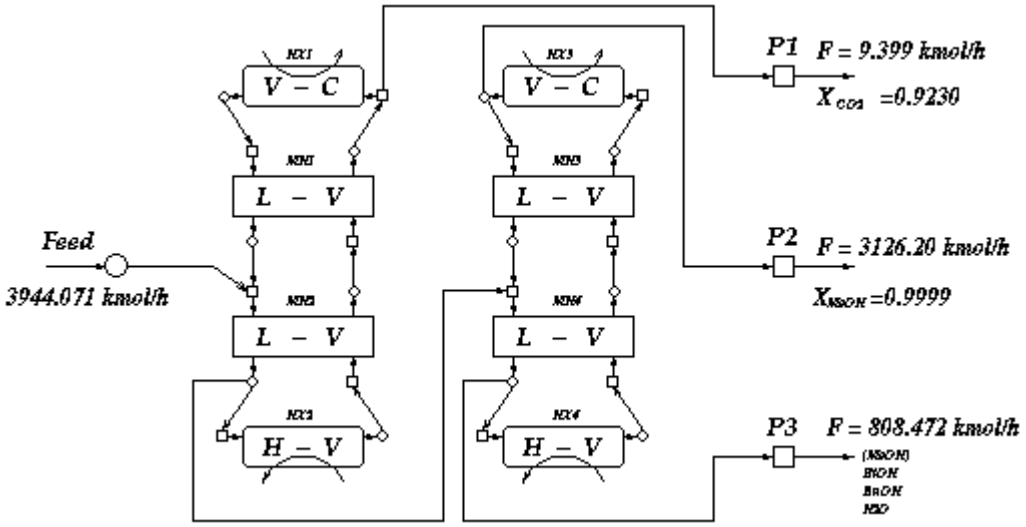


Figure 4 : Result similar to flowsheet alternative 5

5. Conclusions

Task [T1]

What has been accomplished in this task, is a process synthesis prototype tool that

·explores alternative reaction schemes and intermediate process materials
·selects the most appropriate reactor configurations and separation sequences
· expands the process system boundaries beyond the on-site battery limits in terms of the energy generation and the process providing the raw materials
· introduces a temporal aspect to the scope of the design problem by investigating the life cycle potential of the process in terms of energy usage and waste generation.

Furthermore, the above have been studied

· in a multi-objective environment targeting the minimization of the energy usage, the environmental impact and of course the cost
· employing a new process synthesis representation and methodology that is based on elementary physico-chemical phenomena.

5.1.1 Task [T2]

The proposed model has been validated simulating a separation system for a three-component and four-component mixtures, and with the synthesis of a separation system for a four-component mixture. The results of the synthesis study have been compared to the conventional tray-by-tray distillation column model. The main conclusions reached from the validation stage are:

· The mass/heat exchange network representation framework is sufficient to describe physico-chemical phenomena that drive a process and their limitations.

· The same model can result in very different separation systems, without having pre-postulated any particular structure or separation schemes.

· Detailed optimisation of design and operation of particular process units requires further developments and more detailed models.

5.1.2 Task [T3]

This study supports the results of a number of comparisons where a set of different objectives were considered. When the trim loss is minimized without considering other tasks, the over production becomes a problem. Even if we added a term to consider the total number of patterns, the result was still not applicable. This comparison indicates that attention should be paid also on environmental aspects when formulating the objective function. As a result we can say that the objectives 4 and 5 give the best overall results. Furthermore, there is a clear connection between the production time and energy consumption. A very interesting property of the objective comparisons that was discovered was the trade-off between different objectives, which makes the problem a very interesting multiobjective problem.

5.1.3 Task [T5]

The Computer-Aided Design tool-kits are focusing on the application areas characterised by the specific industrial processes studied. The two resulting prototype tool-kits have a broad range of generic applications. At the heart of both developments is a capability for multi-objective mixed-integer non-linear optimisation. It is believed that the software developed in IDEES is the first successful industrial application of such optimisation and the first that has been made sufficiently generic for wide scale application.

5.1.4 Task [T6]

The Case Studies provided by the industrial partners STATOIL, WISAPAK have been defined and are being carried out in order to test and further refine the proposed integrated process synthesis framework. A first sub-task focusing on refinery/petrochemical plant, concentrates on the verification of the synthesis representation part and its corresponding methodology. A second sub-task, dealing with a paper mill, mainly focuses on the site wide and operational aspects in conjunction with the developed numerical techniques. A third sub-

task focuses on the synthesis aspects with respect to flowsheet, energy integration and operability issues. All three sub-tasks involve complex processes with high energy requirements.

Case study 1 : Crude Preheat System - CPERI, STATOIL, IMPCOL.
The heat integration synthesis framework has been applied to the crude oil preheat system at the STATOIL refinery. Heat integration possibilities in the crude preheat system have been modelled and optimised with respect to fuel consumption (cost) and steam production (energy). Preliminary results indicate the potential for substantial improvements in the design and operation, and provide insight on the trade-offs involved. The results have been reviewed and necessary revisions have been identified to improve the existing models.

Case Study 2 : Trim Loss Problem - AAU, WISAPAK, IMPCOL, CPERI
The comparison of different objective functions for the trim-loss scheduling problem is progressing and the application of algorithms presented in a real production environment is underway, so far with very promising results. The developments of this study have been incorporated within a prototype software application currently in use in the WISAPAK paper factory.

6. Annexes

6.1.1 Refereed Publications

Rahim-Ismail, S., E.N. Pistikopoulos, K.P. Papalexandri. *Separation of Nonideal Mixtures based on Mass/Heat Exchange Principles. The Entrainer Selection and Sequencing Problem*. Comp. Chem. Engng., Vol 21S, pp. S211-S216 (1997).

Dimkou, T.I., and K.P. Papalexandri, *A Parametric Mixed Integer Optimization Approach for Multiobjective Problems involving Discrete Decisions.* Paper accepted in ESCAPE-8, Brugge, 1998.

Papalexandri, K.P., D.I. Patsiatzis, E.N. Pistikopoulos and L. Ebbesen, *Heat Integration Aspects in A Crude Preheat Refinery Section*. Paper accepted in ESCAPE-8, May 1998.

Dimkou, T.I. and K.P. Papalexandri, *A Parametric Mixed Integer Optimization Approach for Multi-objective Engineering Problems* Proceedings of 1st Panhellenic Scientific Conference on Chemical Engineering, pp. 541-546, Patras, 1997.

Patsiatzis, D.I., K.P. Papalexandri, S. Rahim-Ismail and E.N. Pistikopoulos, *Synthesis of Separation Systems based on Mass/Heat Exchange Principles.*

Ideal and Nonideal Separations Proceedings of 1st Panhellenic Scientific Conference on Chemical Engineering, pp. 567-572, Patras, 1997.

Pertsinidis A., Grossmann I.E., and McRae G.J., *Parametric Optimization of MILP programs and a framework for the Parametric Optimization of MINLPs* accepted for presentation in ESCAPE-8, May 1998.

Harjunkoski I., Westerlund T., Pörn R. and Skrifvars H. (1997). *Different Solving Trim-Loss Problems with MINLP Methods.* AIDIC Conference Series, Selected Papers of ECCE-1 (accepted).

Harjunkoski Iiro (1997). *Application of MINLP Methods to a Scheduling Problem in the Paper-Converting Industry.* Denmark Technical University – Doctoral Thesis.

6.1.2 Magazine Articles

Finnström Timo (1996). *Optimoinnilla miljoonasäästöt paperinjalostuksessa.* Paperi ja Puu - Paper and Timber Vol. 78/nr. 5/1996

6.1.3 Conference Presentations

Papalexandri, K.P., S. Rahim-Ismail and E.N. Pistikopoulos, *A Multifunctional Process Module for the Synthesis of Combined Reactor/Separation Systems.* Paper presented (poster) at the AIChE Annual Meeting, Los Angeles, 1997.

Pertsinidis A., Stephanopoulos G., and Pistikopoulos E.N, *A Combined Artificial Intelligence-Mathematical Programming Approach in Process Synthesis* First Greek Scientific Symposium in Chemical Engineering, Patras, May 1997.

Rahim-Ismail, S., E.N. Pistikopoulos and K.P. Papalexandri, *Synthesis of Homogeneous Azeotropic Separation Systems based on Mass/Heat Exchange Principles* Presented at the AIChE Annual Meeting, Chicago, 1996.

6.1.4 Papers Submitted / Under Preparation

Papalexandri, K.P. and T. Dimkou, *A Parametric Mixed Integer Optimization Approach for 2-Objective Engineering Problems Involving Discrete Decisions.* Paper submitted to Ind. Eng. Chem. Res. (1997).

Harjunkoski I. and Westerlund T. (1997). *Enlarging the Trim-Loss Problem to Cover the Raw Paper Mill.* Paper submitted to ESCAPE-8.

Harjunkoski I. and Westerlund T. (1997). *Solving Trim-Loss Problems with Variable Raw Paper and Trim-Loss Widths.* Paper under preparation.

Pertsinidis A., Grossmann I.E., *Multiparametric Optimization of MILP programs* to be submitted to Computers and Chemical Engineering, 1998.