ENERGY OPTIMIZATION OF INTEGRATED PROCESS PLANTS

A thesis submitted in partial fulfilment
of the requirements for the Ph.D degree

by

JAN SANDVIG NIELSEN

under the supervison of

Professor Sten Bay Jørgensen
Department of Chemical Engineering
Technical University of Denmark

Production Manager Jens Møller-Birkebæk
KEMIRA Danmark A/S

Mogens Weel Hansen
dk-TEKNIK

Conducted under the Industrial Ph.D programme
Academy of Technical Science
EF443

May 1995/
October 1996

DISCLAIMER

Portions of this document may be illegible electronic image products. Images are produced from the best available original document.

ACKNOWLEDGEMENTS

I would like to thank a number of people who have helped me through this study. First of all the members of the supervisor group - Jens Møller-Birkebæk and Bjarne Christensen for believing in the work, Sten Bay Jørgensen for accepting a mechanical engineer as student and Mogens Weel Hansen for immediate testing of all developed tools.

Further a thank to rest of the people at Kemira who have I have had the pleasure to work with. Especially Henning Møller Jensen for helpful discussion about the process plants. I am also indebted to dk-TEKNIK, who supported my study and granted me two and half years leave from my job.

I would also thank Professor Bodo Linnhoff for letting me stay half a year at the Department for Process Integration at UMIST. The time there has been very stimulating. Thanks also goes to Antonis Kokossis for very fruitful discussions. Rest of the Department also deserves thanks for creating a very pleasant atmosphere.

ABSTRACT

Practical use of advanced design methodologies for energy synthesis of industrial processes has so far been limited. There are several reasons for this. At high conceptual level there are only few tools readily available for practitioners. At detailed level the methodologies are often restricted to problems based on crude simplifications. The problems are thus often fitted to the application and not vice versa. This thesis is directed at the practical aspects encountered in applying efficient synthesis methodologies for real life industrial problems.

A general approach for viewing the process synthesis as an evolutionary process is proposed. Each step is taken according to the present level of information and knowledge. This is formulated in a *Process Synthesis Cycle*. Initially the synthesis is conducted at a high abstraction level maximising use of heuristics (prior experience, rules of thumbs etc.). When further knowledge and information are available, heuristics will gradually be replaced by exact problem formulations.

The principles in the *Process Synthesis Cycle*, is used to develop a general procedure for energy synthesis, based on available tools. The procedure is based on efficient use of process simulators with integrated Pinch capabilities (energy targeting). The proposed general procedure is tailored to three specific problems (Humid Air Turbine power plant synthesis, Nitric Acid process synthesis and Sulphuric Acid synthesis). Using the procedure reduces the problem dimension considerable and thus allows for faster evaluation of more alternatives.

At more detailed level a new framework for the Heat Exchanger Network synthesis problem is proposed. The new framework is object oriented based on a general functional description of all elements potentially present in the heat exchanger network (streams, exchangers, pumps, furnaces etc.). With the new framework more realistic formulation of the synthesis problem can be treated, including temperature dependent stream properties, non-countercurrent heat exchange and complex cost functions. The problems rising from this extended formulation are highly nonlinear and features in general discontinuities in abundance. This makes it difficult to apply standard gradient based optimisation methods to the problem. Therefore, a Simulated Annealing algorithm is proposed to solve the problems. Simulated Annealing has the advantage of being rather insensitive to nonconvex nonlinearities and discontinuities. The proposed framework is implemented in the PC-based synthesis tool *HEN Explorer*.

HEN Explorer is successfully tested against literature problems. For all tested problems *HEN Explorer* successfully finds the better solutions. Especially for complex problems (retrofit, nonconstant properties and tube and shell exchangers) *HEN Explorer* proves superior.

A new concept in nitric acid energy recovery is presented. The process improvement is based on a better utilisation of the high temperature heat release in the process. This is done by enhance the massflow into the integrated tail gas turbine. Massflow increase is realised using a new absorption tower where the cold tail gas absorbs preheated water. The new process is evaluated using the proposed general synthesis procedure. With the new process concept nitric acid can be produced with a specific power production of 326 kWh/t(100% HNO_3). Modern plants typically yields 130 - 150 kWh/t(100% HNO_3) but can be optimised to yield 220-230 kWh/t(HNO_3). The enhanced power production is realised with no changes in the core of the process and should thus only require little further development before the process is mature for construction.

Similar a new route is proposed for energy efficient production of sulphuric acid. Here it is demonstrated that the power production potential for the pressure contact process is higher than for the atmospheric contact process. This is in contrast with previous assumptions. While the atmospheric process has a power production potential of 292 kWh/t(100% H_2SO_4) the pressure process has a potential of 322 kWh/t(100% H_2SO_4). Saturation of the tail gas enhances the potential to 356 kWh/t(100% H_2SO_4).

The proposed methodologies are also used to evaluate Kemira existing processes. While economical feasible energy improvements are limited for the acid processes, a considerable potential for power production in the NPK sector is disclosed. With optimal integration of a gas turbine unit electricity can be produced with a marginal thermal efficiency up to 58%. With the proposed arrangement an operation profit of up to 36 MDKK/yr can be realised with reasonable pay back periods (2 - 5 years).

Finally Kemiras utility system (steam turbines and steam mains) is synthesised for optimal operation. A linear programming model is proposed that finds the optimal operation point based on current energy costs (natural gas, power, district heating) and process steam demands. The model can thus calculate the effective internal steam costs.

RESUMÉ (PÅ DANSK)

Praktisk brug af avancerede metoder til analyse og optimering af industrielle processes energiomsætning har hidtil været begrænset. Der er forskellige årsager til dette. På overordnet konceptuelt niveau er der kun få værktøjer til rådighed for den industrielle bruger. På det mere detaljerede niveau, er de udviklede metoder og værktøjer ofte kun istand til at løse stærkt simplificerede problemstillinger. Det er således ofte problemerne, der må tilpasses metoderne og ikke omvendt. Denne afhandling er rettet mod de praktiske problemer, der optræder når avancerede metoder anvendes til analyse og optimering af reelle industrielle problemstillinger.

Det foreslås at anskue hele optimeringsprocessen som en løbende evolutionær proces. Hvert skridt, der tages sker ud fra den aktuelle viden og information. Dette er formuleret i en *Process Synthesis Cycle*. I starten foretages syntesen på et højt abstraktionsniveau, hvor heuristik anvendes maksimalt (erfaring, tommelfingerregler o.s.v.). Når yderligere viden og information er til stede, bliver heuristikken erstattet af præcise problem formuleringer.

Principperne ved *Process Synthesis Cycle* er udnyttet til at danne en general procedure til energioptimering, baseret på de værktøjer, der er tilgængelige. Proceduren er i høj grad baseret på simuleringsværktøjer med et integreret Pinch analyse værktøj. Den foreslåede procedure er tilpasset tre specifikke optimeringsopgaver (Optimering af Humid Air Turbine kraftprocessen, optimering af salpeter og svovl syre processerne). Med den foreslåede procedure er problemernes dimension reduceret betydeligt og det er således muligt hurtigt at gennemregne mange alternativer.

På et mere detaljeret niveau er der opstillet et nyt strukturelt koncept for optimering af varmevekslernetværk. Det nye koncept er objekt orienteret, baseret på en funktionel beskrivelse af de forskellige elementer, der kan indgå i et varmevekslernetværk (processtrømme, varmevekslere, pumper o.s.v.). Med det nye koncept er det muligt at behandle mere detaljerede problemstillinger. Dette inkluderer temperaturafhængige stofværdier, ikke-modstrøms varmevekslere og komplekse prisfunktioner. De resulterende problemstillinger vil ofte være yderst ikke-lineære og typisk have et utal af diskontinuiteter. Dette besværliggør brugen af gradient baserede optimeringsmetoder. Der er derfor valgt at benytte en metode baseret *Simuleret Udglødning*. Simuleret udglødning har den fordel, at den er forholdsvis upåvirket af ikke-lineariteter og diskontinuiteter. Det foreslåede koncept er implementeret i PC-programmet *HEN Explorer*.

HEN Explorer er med succes afprøvet på en række litteratur problemer. For alle de testede problemer vis *HEN Explorer* sig i stand til at finde de bedste resultater.

Specielt for komplekse problemstillinger (retrofit, temperaturafhængige stofværdier o.s.v.) viste *HEN Explorer* sig overlegen.

På den mere udviklingsmæssige side er der udviklet en ny salpetersyreproces med forbedret energiudnyttelse. Processen er forbedret gennem en bedre udnyttelse af den varme, der afsættes ved høj temperatur. Dette er gjort ved at øge masseflowet ind til den integrerede retgasturbine. Masseflowet er øget ved at benytte en ny absorptionskollonne, hvor den kolde restgas absorberer foropvarmet vand i modstrøm. Den nye proces er optimeret ved hjælp af den udviklede generelle optimeringsmetode. Med det nye koncept kan salpetersyreprocessen specifikt producere 326 kWh/t(100% HNO_3). Til sammenligning yder moderne anlæg typisk 130 - 150 kWh/t(100% HNO_3) men kan optimeres til at yde 229 kWh/t(100% HNO_3). Den øgede kraftproduktion opnås uden at ændre på kernen af processen. Derfor skulle det foreslåede koncept med beskeden videreudvikling være klar til kommerciel brug.

På tilsvarende vis er der udviklet en ny proces til energieffektiv produktion af svovlsyre. Det er demonstreret at potentialet for kraftproduktionen på et tryksat svovlsyreanlæg er højere end på et tilsvarende atmosfærisk anlæg. Dette er i modsætning til, hvad der hidtil er antaget. Ved den atmosfæriske proces er det muligt at opnå 292 kWh/t(100% H_2SO_4) mens der for den tryksatte kan nås 322 kWh/t(100% H_2SO_4). Ved befugtning af restgassen kan potentialet for den tryksatte proces øges til 356 kWh/t(100% H_2SO_4).

De udviklede analysemetoder er også anvendt til Kemiras eksisterende processer. Mens økonomisk mulige forbedringer er begrænset for syre processerne, er der et stort potentiale for kraftproduktion i NPK sektoren. Ved optimal integration af et gas turbine anlæg er det muligt at producere el med en marginalvirkningsgrad på op til 58%. Med det foreslået system er det muligt at opnå et årligt driftoverskud på op til 36 Mio.Kr/år med en rimelig tilbagebetalingstid (2 - 5 år).

Endelig er Kemiras energiforsyningssystem (damp turbiner, gas turbine, dampledninger m.m.) optimeret med henblik på optimal drift. En linear optimeringsmodel er opstillet. Ved løsning af denne kan det optimale driftspunkt findes baseret på aktuelle energipriser (naturgas, el og fjernvarme) og på procesdampbehovet. Modellen kan således også benyttes til at beregne de effektive interne dampudgifter.

Contents

Papers

Nielsen J.S.; Energy Optimisation by Simulated Annealing, Paper presented at ASME Winter Annual Meeting, New Orleans, November (1993).

Nielsen J.S., V. Briones-Vallejo and A.C. Kokossis; An Integrated Framework for the Optimal Design of Heat Recovery Network, Paper presented at AIChE annual meeting, San Francisco, November (1994).

Nielsen J.S. and M.W. Hansen; Improved Synthesis of the Nitric Acid Process, Paper presented at International Mechanical Engineering Congress and Exposistion, San Francisco, November (1995).

Appendices

0
INTRODUCTION

"People would rather live with a problem they cannot solve than accept a solution they cannot understand" (Woolséy and Swansson, 1975).

0.1 The aims of this work.

This thesis presents a practical approach to the various problems encountered at a complex industrial site. The main aim is to provide/apply methods that are able to carry the synthesis from an abstract conceptual level to a final practical level, with as much transparency as possible. A vast amount of work within *Pinch Analysis*, *Exergy Analysis* and *Mathematical Programming* has aimed at methodologies for optimization of various part of the synthesis problem. It is the intention of this work to learn as much as possible from these works, to avoid reinventing the wheel - so to speak. An inherent aim is therefore to review existing design technologies and to put these into perspective for general use.

The scientific challenge that is encountered in this thesis is handling of the complex nonlinearities and discontinuities that arise when formulating realistic industrial problems. The combinatorial aspect is of especially importance when looking at the synthesis of heat exchanger network. A specific objective is to develop a synthesis strategy for assessing the complex constraints that can occur in designing industrial heat exchanger networks.

It is further the aim to demonstrate how different approaches can be applied to optimize the energy situation at Kemiras Fertliser site in Frederica. Based on the experience from the plant analysis the different design technologies are to be evaluated in terms of practical usages. Special attention will be paid the energy intensive processes (nitric acid process, sulphuric acid process and NPK process).

0.2 Outline of this work.

This thesis comes in two parts. In the first part (chapter 1 through 7) the theoretical aspect of process synthesis is treated, while in the second part (chapter 8 through 14) practical aspect and implementation for specific problems are handled.

In chapter 1 the general aspect of process synthesis will be outlined based on a literature survey, followed by a proposal of a new concept - *Process Synthesis Cycle*. In chapter 2 the energy aspect of process synthesis is extracted and an overview of different approaches is given. Chapter 3 treats *Pinch Analysis* in particular. This

chapter gives a thorough review of state of the art within Pinch Analysis. Chapter 4 treats the *Mathematical Programming* approach to Heat Exchanger Network (HEN) problem. In chapter 5 *Simulated Annealing* is introduced as a general approach for global optimisation of complex problems. This also includes a description of Simulated Annealing applied to the HEN problem. This is pursued in chapter 6 where a *New Framework for the HEN problem* is proposed based on object oriented programming and Simulated Annealing. The proposed framework is implemented in *HEN Explorer*. In chapter 7 a simple generic procedure for general energy synthesis is proposed.

HEN Explorer is tested for a range of different literature problems (chapter 8). This includes grassroot and retrofit design. In chapter 9 the general procedure for energy optimisation has been adopted tailored to a specific problem (Humid Air Turbine power plant). This chapter illustrates how targeting methods can be applied in a simple fashion to provide fast process evaluation. Chapter 10 presents a new process for nitric acid production (*Saturated Nitric Acid plant*) which is showed to increase the energy efficiency substantially. The proposed process is optimised using the general procedure outlined in chapter 7 and with use of *HEN Explorer*. Chapter 11 treats energy improvements in the nitric acid sector, while chapter 12 treats the sulphuric acid process. In chapter 13 the aspect of performance degradation and monitoring is outlined. Integration of gas turbine in the NPK sector is evaluated in chapter 14, where a large potential saving is identified. Finally chapter 15 treats the possibilities of improving the site utility system. The work is concluded in chapter 16.

1
INTRODUCTION TO PROCESS SYSTEMS ENGINEERING

In this chapter the general approach to process synthesis is discussed based on a literature review.

The understanding of unit operations is the cornerstone of virtually all engineers working with process plants. Most of today's processing plants are, however, becoming more integrated in order to enhance production efficiency in terms of energy, raw material and disposal. It is therefore evident that system engineering is to become more and more important for chemical engineers. Process systems engineering is oriented towards the understanding and design of a system of unit operations at the flowsheet level (Gundersen, 1991).

Process Synthesis is often used as a general term regarding the design of processing system ranging from individual unit operations to complex chemical plants. In this work the term "Process Synthesis" will mean the work towards better system design of the processing system.

Another commonly used term for process system engineering is *Process Integration*. Unfortunately this term is widely used as a synonym for Heat Integration and in some cases for a specific method (Pinch analysis). In this thesis therefore the use of the term Process Integration will be omitted.

1.1 The role of process design work.

The process design problem is virtually always a part of a total managing problem. The overall design decisions, therefore, normally starts long before it shows up at the process engineers table.

The managing work involves not only the process synthesis but also project organisation, manufacturing organisation, sales and maintenance. Lately, focus on life cycle has also included the final disposal of the plant as a matter of importance. In fact the value of process synthesis is dependent of what elements are included in the specification of the synthesis problem. The elements included can basically be placed in two categories. They can either be constraints or they can be included in the objective of the synthesis. A typical example is environmental considerations. Emission can for example either be treated as a constraint (maximum concentration) or included in the objective function. Simply ignoring these elements can result in inferior solution if an expensive treatment plant has to be applied subsequently.

This is leading to a basic acknowledgement:

> Process plants operates under the conditions and influence of the surrounding world. The result is that process plant optimisation is bounded, not only by thermodynamics, but also by economics, environment, legalisation authorities, individual preference and politics.

Not recognising this problem setting could cause great disappointment and a great lost of work. This should, however, not discourage people to continue developing and refining the process synthesis steps. Actually the above acknowledgement should be used to enforce the role of rational improvements and to fight for acceptance of process synthesis as a central and important task.

1.2 Process synthesis and process hierarchy.

To perform process optimisation studies it is crucial to acknowledge the hierarchy of the processes. Only when the process hierarchy is understood the engineer can carry out reliable process design calculation. A very illustrative way of expressing the process hierarchy is the onion diagram proposed by Linnhoff (1983).

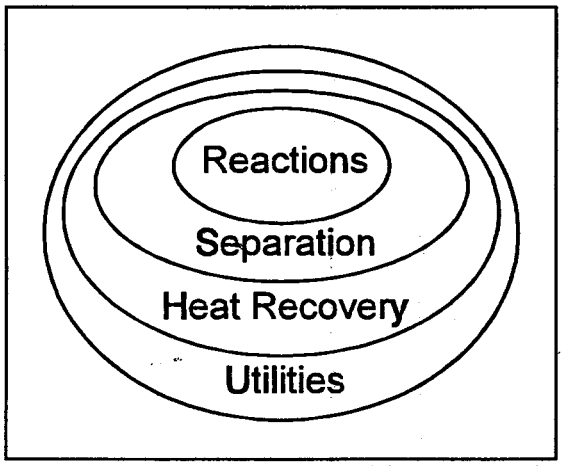


Figure 1.2.1 The onion model proposed by Linnhoff (1983).

The onion model indicates that process design should be starting with the heart of the process - the chemical reactions. Decide what reaction schemes there should be used to transform the raw material into the wanted product. After this is achieved, the next step is to purify or separate the reaction products. This is done by selecting and sizing separation equipment, recycling streams etc. The third layer is the heat exchanger network. The heat recovery task is to recover heat supplied or formed during the processes and thus diminish the total energy demand. Finally the last layer of the onion is the utility system. The function of the utility system is to supply the total system with sufficient energy, process water etc.

A most important Feature of the onion model is that it clearly emphasises the importance of downstream analysis. I.e. a change in reaction path influences the outer onion layers and not vice versa. However, the optimum design of the reactor can not be achieved without consideration of the outer layers.

The term *optimum system* makes only little sense in the literary meaning because the industrial reality is limited resources, limited knowledge and incomplete information. The process synthesis can thus be defined as the activity of generating design alternatives and selecting the best one on incomplete information (Westerberg, 1989). When using the phrase's optimum design and optimisation in this chapter, it is thus to be understood as choosing the best design on limited information.

Another way of illustrating the process interactions is proposed by Papoulias and Grossmann (1983) and adopted in similar forms by others (e.g. François and Boris 1989). This is based on the assumption that a total processing system can be regarded as an integrated system consisting of three main components.

1. Chemical plant
2. Heat recovery network
3. Utility plant

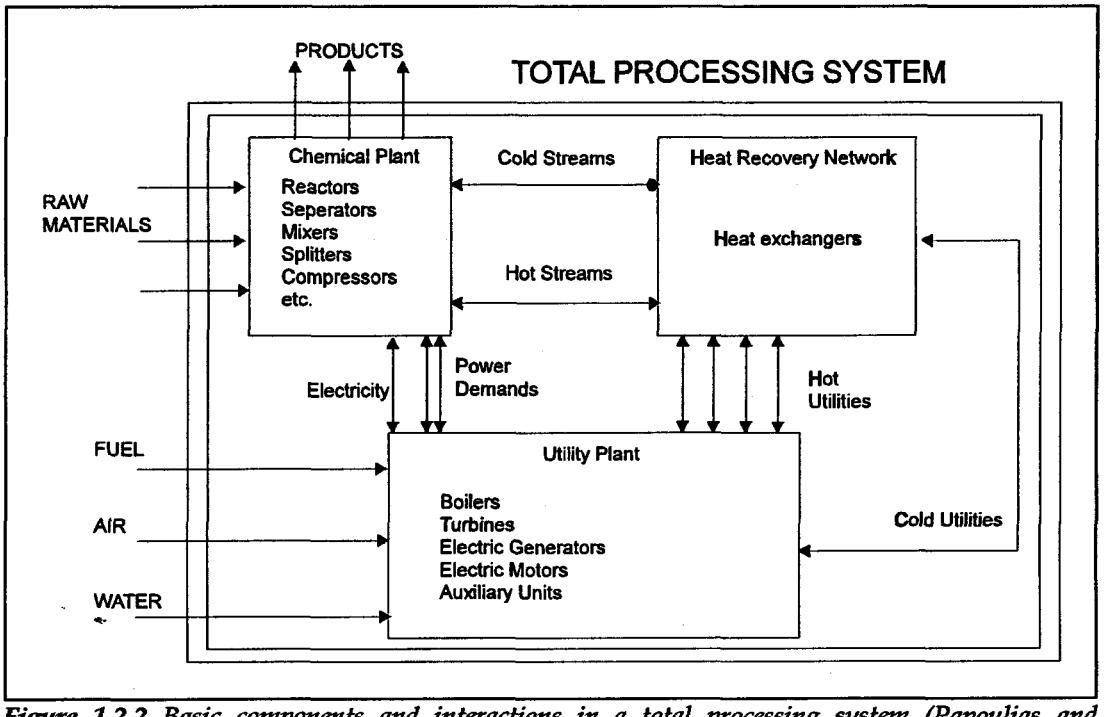


Figure 1.2.2 Basic components and interactions in a total processing system (Papoulias and Grossmann 1983).

Again understanding the nature of interaction is crucial. The interactions among the chemical with the heat recovery network are the process streams that require heating or cooling. Interactions between the chemical plant and utility system are the electricity and power demands required in the chemical plant. Finally, the interactions between the heat recovery network and the utility system are the hot and cold utilities required for providing the necessary heating and cooling in the heat recovery network.

Together the onion model and the interaction model form are useful for understanding the hierarchy of process system. The onion diagram delivers the fundamental understanding of process dependencies while the interaction model delivers a functional description of the problem that can be used in the setting up solution procedure for the problem.

Árva and Csukás (1988) propose to divide the process synthesis problem into three basic tasks.

1. The representation, which should clearly generate the possible variants.
2. The sufficiently quick and exact evaluation of investigated objects.
3. The strategy, which is able to select the better systems upon the realisation of a little part of them.

It is important to notice the level of detail. This is one of the key questions that arise when looking at large processing plants. If a rigorous representation is used, the number of equations is huge, and in practice impossible to handle. Therefore, detailed representation should only be used in part of the system. This leave us with a paradox that is central in process synthesis. The system behaviour is dependent on a detailed process description and the detailed process description is dependent of the total system. One of the most important element of process synthesis is to select some kind of intermediate description. An often used term for an intermediate description is *Conceptual design* (Mizsey and Fonyo, 1990; Douglas, 1988).

There are several approaches to synthesis of total processing system. These can mainly be divided into

1. Iterative optimisation using decomposition into the main components (f.x. as suggested in the interaction model). In each step each component is optimised starting from the onion centre. Interaction is basically taken care of by engineering insight and/or targeting methods.
2. Simultaneous optimisation by setting up a superstructure that cover different processing schemes. The optimisation is here normally done by algorithmic methods.

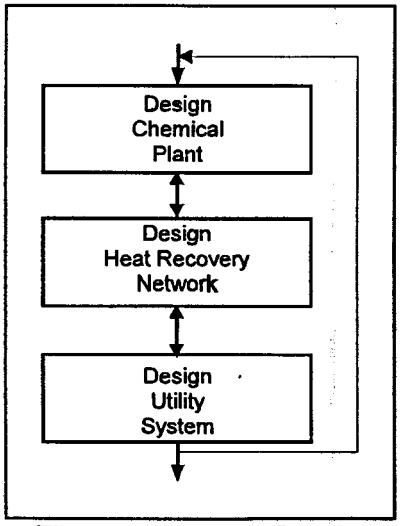


Figure 1.2.3 Iterative optimisation scheme for total processing plant synthesis.

The iterative procedure typically starts with an initial chemical plant design. This design gives fixed process streams that are followed by an initial heat recovery network design. Given a fixed heat exchanger network the utility demand is fixed and the utility system can be (sub)optimised. Now the network can be changed in order to optimise the combined heat recovery network/utility system. When this is optimised the chemical plant design can be modified and new optimum recovery network/utility system can be evaluated. The iteration scheme is outlined in Figure 1.3.

In practice the outer loop of the iteration scheme is normally considered only for few process alternatives and in many cases the chemical plant design is assumed fixed. This is particularly the case in retrofit studies. Also each step in the iteration scheme is preoptimised by assumption of fixed energy costs etc. One example is optimisation of the heat exchanger network assuming constant energy cost. The major force of the iterating approach is that it is possible to reduce the total problem into smaller manageable

problems. Having in mind that the problem information is normally incomplete the iteration approach allows for human interaction after each step.

The simultaneous approach uses a superstructure setting up all relevant processing alternatives. This superstructure is formulated so that it can be optimised using advanced mathematical programming. From a mathematical point of view the simultaneous approach is superior to the iterative approach. However, the simultaneous approach demands a priori knowledge of all possible interaction. From the fact that process synthesis is characterised by its large combinatorial nature this demand can cause severe problems. According to Douglas (1988) a synthesis problem can have 10^4 - 10^9 process alternatives. Therefore using the simultaneous approach does not prevent the need for a preliminary screening of alternatives.

There is no evidence that one approach is superior to the other. Mizsey and Fonyo (1990) conclude that different design steps should not be solved by a single approach and that each type of approach has its own proper place in the complete design process.

In this thesis the main objectives are to develop and apply methods for process synthesis from an energy efficiency point of view. Therefore, in the subsequent chapters the main stress will be laid on the energy aspects of processing plants. As outlined in Figure 1.3 the heat recovery network and utility system cannot be regarded isolated. Therefore, the interconnections between the heat recovery network and the "chemical" processes will be examined when necessary.

1.3 Process hierarchy and synthesis - Discussion.

Process synthesis must be regarded as an evolutionary human process where the understanding and feeling for the system are steadily increasing. This understanding should also reflect on the approach for identification of improvements.

Because of the high level of uncertainties normally associated with process synthesis a high level conceptual description is usually enough for the initial screening among process alternatives. The conceptual description should therefore be concentrated on including structural design. At the high level conceptual design stage it is necessary to introduce several assumptions. At subsequent stages these assumptions must be re-evaluated. If the assumptions have failed it is necessary to return to the high level conceptual design stage. Process synthesis is thus an iterative process. The challenge is to reduce the number of iterations by systemising the synthesis process.

A new way of viewing the general *process synthesis cycle* is outlined in Figure 1.3.1.

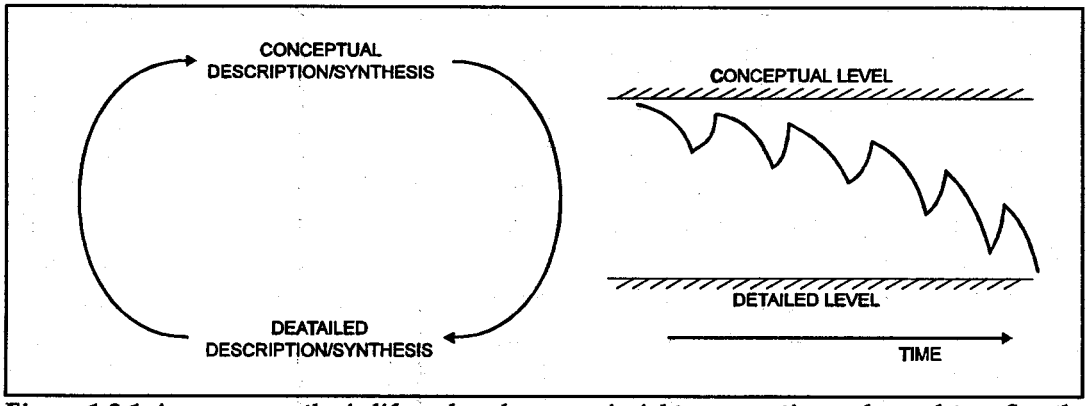


Figure 1.3.1 A process synthesis life cycle, where new insights are continuously used to refine the synthesis framework.

The process synthesis cycle starts with a rough (conceptual) representation of the system to be evolved. Using this rough model the system can be evaluated quite easily and more information can be gathered where necessary. When more knowledge of the system is available more elaborate model can be used to get more precise results. When the system is finally synthesised with a more or less detailed model a rigorous process simulation can be carried out in order to refine the results and to perform sensitivity analysis.

The time factor is worth mentioning here. Probably most industrial process synthesis projects are limited by time resources. This limitation reinforces the need for good and simple conceptual design methods for initial screening among alternatives. This time limitation often results in a rather anarchistic approach, where different design methodologies (rules of thumbs, pinch analysis etc.) are applied uncoordinated. This could cause in a inefficient use of design technologies. This important matter is unfortunately often ignored.

Another side of the industrial aspect is the transparency of the approach. If the approach is too complicated the approach is doomed on beforehand no matter how well thought out the approach is. It is very important that all steps of the approach are well defined and easy to perform if the objective is to generalise the approach.

When it comes to choose between iterative approaches based on 1) hierarchical insight and targeting methods and 2) the simultaneous/algorithmic approach it is obvious that both approaches have their advantages and pitfalls. It is recently been illustrated by Nielsen et al. (1994) that by combining the approaches it is possible to take advantage of the complementary features of the approaches. This is discussed in detailed by Nielsen et al. (1994, enclosed in appendix).

2
ENERGY OPTIMISATION TASKS AND APPROACHES

As mentioned earlier the energy aspect of the process synthesis cannot in general be regarded as an isolated task. In many cases the interface between the core process and the energy transfer system is of importance. Ignoring this can cause failure to find major improvements. This issue will be discussed further in chapter 3.

The process design work can be split in several initial decisions. What type of project and what kind of process.

1)	Task	Retrofit design, Grass root design.
2)	Process operation type	Batch processes, Periodic processes, Continuous processes.

These are normally the preliminary questions to be considered. For retrofit design the process type is normally not to be changed while in grass root design the decision between continuous and batch process is normally free.

There are also several levels of optimisation tasks. From totally new process concepts to minor auxiliary system optimisation. The depth of the analysis work must always be in accordance with the goal of the analysis. However, the onion and the interaction model should always be kept in mind.

In this thesis the major stress will be laid on the thermodynamic aspect of continuous processes. The inner layer in the onion model (reactor and separation system selection) will basically be assumed fixed.

The approaches for energy optimisation can be grouped in the following way:

- Rules of thumb, prior experience
- Thermodynamic and physical based methods (exergy, pinch technology etc.)
- Simulation based trial and error search
- Model based optimisation (Mathematical programming)
- Expert system

Usually more than one approach is used in the optimisation process. In most cases prior experience and rules of thumbs will be needed to cut down the overall engineering time.

2.1 Second law based methods for heat integration.

Thermodynamic based methods for increasing the energy efficiency of integrated process plant are basically based on minimising the entropy generation according to the second law of thermodynamics. Exergy has been widely accepted as a good conserved quantity for describing the quality of energy (e.g. Reistad and Gaggioli 1980). It is however evident that exergy as an indicator for energy quality can be misleading. This is demonstrated by Alefeld (1988) by comparing thermodynamic cycles (heat engines and heat pumps) with entropy balances and exergy balances. The key point in the demonstration is that a second law efficiency should only be dependent of the parameters that the process really depend on. This is in contrary to the exergy efficiency that depends on the surrounding conditions. He instead suggests a method based on entropy generation.

The pinch method is also a second law based method although it's not as general as the exergy and entropy based methods. It does not apply to for example chemical reactions and mass transfer but to processes that can be described by heat sources and heat sinks (Linnhoff 1993), including evaporators, distillation columns, heat engines and heat pumps.

The thermodynamic methods can now be placed in a hierarchy with second law as the base.

Methods based on entropy generation. Calculation of entropy generation in each process unit. The basic assumption is here that minimum entropy generation gives maximum energy efficiency. The scope is all thermodynamic processes.

Methods based on exergy losses. Calculation of loss in working ability in each process unit. The basic assumption is that minimum exergy loss yield a maximum energy efficiency. The scope is primarily heat exchange and working machines.

Pinch method. The pinch method is based on the concept of exergy minimisation in heat transferring processes by minimising the average log mean temperature differences in the total heat exchanging system. The scope of pinch analysis is processes that can be described by heat sources and heat sinks. The pinch method will be described thoroughly in a later chapter.

2.1.1 Second law of thermodynamics.

The energy transformation is bounded by the first law of thermodynamics that says that energy is conserved in any ordinary processes. The first law is thus a quantitative statement pointing out that no energy vanishes. It is, however, well known that the changes between the two energy forms heat and work are restricted by other bounds. One unit of heat is not equivalent to one unit of work. It is also well known that heat exchange between two bodies always takes place from the hotter to the cooler body.

It follows from the above that it is necessary to describe energy not only by quantity but also by quality. This is concentrated in second law of thermodynamics. The second law of thermodynamics can be formulated in various ways. Two of the more common (Smith and Van Ness 1987) are the statements

No apparatus can operate in such way that its only effect (in system and surroundings) is to convert heat absorbed by a system completely into work.

No process is possible which consist solely in the transfer of heat from one temperature level to a higher one.

The classical approach to the second law of thermodynamic is based on the study of heat engines. Essentially a heat engine absorbs heat from a high temperature level (Q_H) and release heat at a low temperature level (Q_C) under production of work (W). The produced work is given by

$$W = |Q_H| - |Q_C| \tag{2.1}$$

The thermal (first law) efficiency of the process can be defined as

$$\eta \equiv \frac{net\ work\ output}{heat\ input} \tag{2.2}$$

or

$$\eta = 1 - \frac{|Q_C|}{|Q_H|} \tag{2.3}$$

For reversible cycles

$$\eta = 1 - \frac{T_C}{T_H} \tag{2.4}$$

known as the Carnot-Kelvin formula with temperature in Kelvin.

The two previous equations can also be stated as

$$\frac{Q_H}{T_H} = \frac{-Q_C}{T_C} \tag{2.5}$$

when the sign convention for heat absorption is positive and for heat release negative.

Based on these considerations the entropy S can be defined

$$dS = \frac{dQ_{rev}}{T} \tag{2.6}$$

$$\Delta S = \int \frac{dQ_{rev}}{T} \tag{2.7}$$

As for the previous equations the quantities dQ_{rev}/T and thus also S sum to zero for reversible processes.

Entropy is useful because it is a state function and thus independent of the process path. From the process data (temperature, pressure and composition) the entropy and enthalpy increases can be evaluated by

$$\Delta S = \dot{m} \int_{T_1}^{T_2} \frac{C_p dT}{T} \tag{2.8}$$

and

$$\Delta H = \dot{m} \int_{T_1}^{T_2} C_p dT \tag{2.9}$$

A quick way of calculating the entropy changes from known values of enthalpy changes is proposed by Linnhoff (1983).

Assuming constant C_p the above equations give

$$\frac{\Delta S}{\Delta H} = \frac{\int_{T_1}^{T_2} \frac{dT}{T}}{\int_{T_1}^{T_2} dT} = \frac{\ln\left(\frac{T_2}{T_1}\right)}{T_2 - T_1} \tag{2.10}$$

This equation demonstrates a general approach. They allow for calculation of entropy changes as a function of enthalpy changes and temperatures. For industrial plants delivered by contractors, it is normal to supply data on enthalpy changes and operating conditions but NOT on entropy data and details on compositions. In such cases the correlation (2.10) can be very useful for second law analysis.

In many second law analyses the thermodynamic performance of a process unit is judged by its second law efficiency or second law loses (e.g. exergy loss). The second law efficiency can be defined in various ways. One of the more frequent is based on the exergy concept.

$$\eta_{ex} = \frac{Recovered\ exergy}{Supplied\ exergy} = 1 - \frac{Exergy\ loss}{Supplied\ Exergy} \tag{2.11}$$

The exergy E quantity for a given state is calculated as the amount of the work ideal obtainable when going to the surrounding state. For a heat transfer process with constant temperatures, the Carnot efficiency can be used (eq. 2.4) for calculating the exergy content for each side of the exchanger.

$$E_{Hot} = \frac{Q}{1 - \frac{T_0}{T_H}} \tag{2.12}$$

$$E_{Cold} = \frac{Q}{1 - \frac{T_0}{T_C}} \tag{2.13}$$

The exergy efficiency for a heat exchange process can thus be calculated as

$$\eta_{ex} = \frac{E_{Cold}}{E_{Hot}} = \frac{1 - \frac{T_0}{T_C}}{1 - \frac{T_0}{T_H}} \tag{2.14}$$

The primary reason for establishing a second law efficiency is to get an unmistakable index of quality of the system (Valero and Royo, 1992). The second law efficiency can be calculated for the whole system or for an individual unit.

It is important to notice that exergy efficiency compares real performance with ideal performance. Therefore an exergy efficiency of unity will usually need infinitely large equipment and infinitely many equipment stages.

2.1.2 Exergy and entropy based methods.

Although the second law is widely accepted for analysis of thermal processes, only limited general suggestion is made on how to increase the thermodynamic efficiencies of thermodynamic processes. The most widespread guideline is to look at the biggest lost first (Gaggioli and Petit 1977). It is however also widely accepted that such guidelines are fallible. From various second law or exergy analyses (e.g. Gaggioli and Petit 1977, Valero and Royo 1992, Rosen 1992, Woudstra and Woudstra 1993) the common approach is to calculate a thermal second law efficiency for each component in the system and then try to maximise all of them. There is unfortunately no widely accepted general method on how to maximise these efficiencies. To complicate it even further, it is in most studies necessary to distinguish between avoidable and

inevitable losses. This can be due to reaction kinetics, equipment limitations and so on. Still there is no doubt about the potential of the second law analysis and research in second law analysis is still intense especially in the mechanical engineering society (see e.g. Boehm 1992 and Richter 1993).

Second law analysis can be carried out in different ways. Unfortunately the majority of the recorded second law based projects is poorly documented and the conclusion often of to general character. Common for most analysis is the calculation of exergy losses in the flowsheets. Only few authors apply detailed methods for minimising the total exergy loss while the majority uses the exergy loss distribution as vague guidelines for identifying potential energy improvements. A typical conclusion (Rosen 1992) is "Efforts to increase plant efficiency should focus on reducing exergy losses since these losses, unlike energy losses, are a direct measure of the lost potential for electricity generation" and further "This study, by using exergy analysis in addition to energy analysis, has provided an improved understanding of the thermodynamic performance of an IGCC (Integrated Gasification Combined-Cycle) power plant. Insights not directly obtainable with only energy analysis, have been acquired. This enhanced understanding may provide the basis for improvements in the design of the IGCC plant considered and its optimisation".

Only a few authors have proposed a detailed method for flowsheet optimisation by second law. One promising approach used by some authors, however, is the thermoeconomic or exergoeconomic approach (von Spakovsky and Evans 1987, 1990; El-Sayed 1992). In the thermoeconomic model, operating cost are based on the Second Law quantities that each component requires to perform its function. Component functions relate the entropy generated in each physical process to the Second Law quantities that each component buys from/or sells to the rest of the system in order to satisfy the Second Law and overcome irreversibility's present in each cycle (von Spakovsky and Evans 1990). These thermodynamic operation costs are balanced with the capital costs of equipment which are formulated mathematically. These costs vary with changes in the thermodynamic operation of the system. This balancing results in a mathematical objective function. The objective function can be solved, subject to various constraints (thermodynamic, material a.o.) for getting an optimum set of performance variables. The procedure is first to decompose the flowsheet into components each with one primary function. In this way, each component in the system consists only of its functions, each function's product, and all the input required for the performance of its functions.

The general set of equations rising from a thermoeconomic analysis consists of an objective function based on costs of second law quantities needed for each component and capital cost calculated from decision variables. The constraints are the mass and energy balances for the system calculated from the decision variables.

The second law quantities can be exergy. However, von Spakovsky and Evans (1990) suggest using a quantity that they defined essergy. This quantity applies to nonequilibrium states. They note that other measures such as exergy, available energy etc., are simply equilibrium cases.

Von Spakovsky and Evans (1990) apply a Lagrange Method for solving the set of equations.

The thermoeconomic approach has so far been demonstrated on power cycles with seemingly good results (El-Sayed 1992, Price 1993). It is however not evident that the method can be transferred to general energy optimisation of industrial process plants. While it makes good sense to compare real behaviour with ideal behaviour in power cycles this can be unfruitful in processing system where many practical considerations means that comparing with the ideal performance in many cases only make little sense.

2.1.3 Exergy and entropy based methods - Discussion.

Exergy based analysis clearly gives the process designer clues of where to look for energy improvements. It is however important to notice that these methods only give clues and not distinctive guidelines. The widely used approach to look at the biggest exergy loss first may in many cases be useful but in general all clues must be investigated in order to identify the true inefficiencies.

One of the major disadvantages with exergy based methods are that they are dependent of the state of the environment. In many case studies much of the emphasis has been laid on defining the environment (e.g. Woudstra 1993). This along with the difficulties in defining the second law efficiency of individual units can make it very confusing to carry out exergy analysis. This is probably also the reason for the virtually non existing industrial use of exergy analysis.

Since most of the proposed methods are based on a flowsheet evaluation of exergy losses they are heavily dependent of the initial flowsheet layout. In thermoeconomics, for example, the initial plant network is broken into subsystems where capital is traded of for exergy costs. It demands a reasonable a priori knowledge of the final solution to find the correct exergy costs. This knowledge can be obtained from an initial flowsheet, which seems to be the traditional approach. With this approach it seems likely that the approaches will limit themselves from major process changes. This limitation enhances the impression that exergy analysis has proven best for systems with a well described flowsheet layout (e.g. power cycles, Kolas 1985).

A further obstacle for industrial use of exergy based methods is the absence of commercial design tools.

2.1.4 Second law and pinch analysis.

One of the most successful implementations of the second law of thermodynamics is the *Pinch analysis* (Linnhoff 1982). The pinch analysis takes its base in the *Process Composite Curves* (Hohmann 1971, Linnhoff 1982) figure 2.1a representing the minimum heat and cooling demand (described in detail in chapter 3). If this curve is transformed from temperature axes into Carnot efficiency axes, figure 2.1b (Linnhoff 1989), the shaded area is equal to the minimum exergy loss. With the pinch method it is actually possible to determine the minimum exergy loss, assuming that no heat

engine or heat pump are used (Linnhoff 1989). This is the unavoidable exergy loss for a given heat exchange process.

This gives important insight compared to traditional exergy analysis where the amount of unavoidable exergy loss is unknown. By using the information from pinch analysis it is possible to compare the real exergy loss with the unavoidable exergy loss. This gives a better basis for comparison.

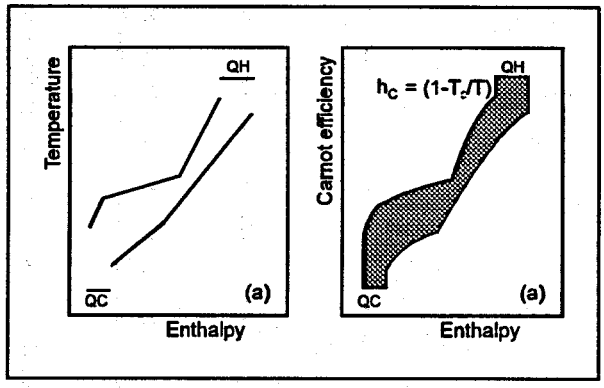


Figure 2.1.1. T,H and η_C curves.

2.2 Simulation based trial and error search.

With the advance of commercial process simulators such as ASPEN, HYSIM etc., it has become possible to perform rigorous process simulation applying complex thermodynamic and physical property models. For the design engineer the process simulator is an excellent tool for quick evaluation of improvement ideas. Process optimisation by trial and error of different ideas have the inherent advantage, that the results are almost immediately validated. With process simulators several alternatives can be evaluated in limited time.

Most simulation packages also have sizing modules for detailed design of process equipment (heat exchangers, columns etc.) taking into account material constraints, equipment efficiencies etc.

Several simulators even have optimisation modules allowing the engineer to optimise a set of design variables in order to optimise a given objective function. These optimisation modules, however tend to be computational expensive.

Simulation based optimisation in general lacks the ability of configurational optimisation. This lack normally restricts the user to evaluate a finite number of process alternatives.

The optimisation strategy when using process simulators is first to construct one or more feasible flowsheets based on previous knowledge. Thereafter several design variables are varied to increase the energy efficiency. Finally a sensitivity analysis can be carried out by varying several parameters (inlet conditions, heat exchanger fouling etc.).

2.3 Model based flowsheet optimisation.

Model based flowsheet optimisation is the approach where the flowsheet problem is formulated in a mathematical way and the problem solved by numerical methods. This

approach is also denoted *The algorithmic approach* (Mizsey and Fonyo 1990) and *Hierarchical Aproocah* (Conceptual design) when applied to an intermediate representation of the flowsheet (Mizsey and Fonyo, 1990; Douglas, 1988).

From a conceptual viewpoint the synthesis problem can be formulated as a combined discrete and continuous optimisation problem which mathematically - in general - gives rise to a Mixed Integer Non-linear Programming (MINLP) problem. To complicate it even further the number of possible structures of the optimum flowsheet is not known in priori.

The most extensive work for setting up and solving the flowsheet equations is probably done by the groups from Carnegie-Mellon University (Biegler 1988, Papoulias and Grossmann 1983a-c, Lang et al. 1988, Westerberg 1980 and Armager et al 1992) and Princeton (Floudas 1989, Ciric 1989) although a lot of other research communities also contribute to the area.

From the previous chapters it is well recognised that energy optimisation cannot be isolated from the total design process. With less expensive energy, more will be used to improve product conversion and vice versa. The overall process design problem is sufficiently complex that many methods propose to decompose the master problem into a sequence of design problems, with energy integration typically being the last (Westerberg 1992). This is accordance with the onion diagram mentioned in chapter one. Since heat integration does affect the earlier decision there is a need for a step that allows for the earlier decision to be altered based on the results developed later on. Therefore most recent methods are based on a stage wise approach where the heat integration effect on initial decisions is evaluated.

A major task of total flowsheet optimisation is to embed the possible process structures. This is done by a so-called *Superstructure*. It's important that the superstructure actually cover the necessary solution space. The superstructure approach was proposed in the late 60's by Ichikawa (Westerberg 1992). In these early approaches, every unit in a superstructure received input from the output of every other unit. Split factors between every unit allowed fractions to be directed to any units. The problem with the early formulation was that it did not allow binary variables to switch units of or on. Later work by Grossmann and co-workers (Papoulias and Grossmann 1983a-c, Grossmann and Sargent 1978b, Grossmann 1992) has extended the formulation to take into account the binary variables.

In figure 2.2 (Westerberg 1992) part (a) represents a superstructure for one stream meeting three other streams to exchange heat. Part (b) shows a substructure in which it meets streams 1 and 2 in parallel and then meets stream 3. (c) shows the substructure in which it exchanges in series with streams 2, 1 and 3.

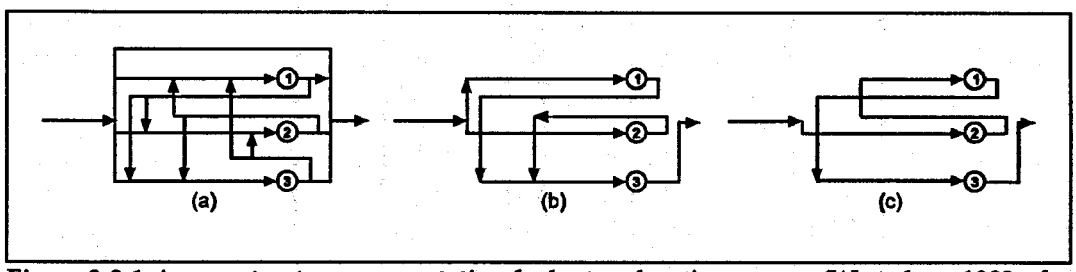


Figure 2.3.1 A superstructure representation for heat exchanging process (Westerberg 1992 after Floudas et al. 1986). (a) full superstructure, (b) and (c) embedded structures.

The superstructure can thus be used to imbed several possible structural solutions. The superstructure approach for heat exchanger network synthesis will be further explained in chapter 4 together with the mathematical methods applied to solve the resulting MP problem.

2.4 Other approaches.

Few other approaches for process synthesis have been proposed. One of them is knowledge based synthesis using an expert system. Stephanopoulos (1990) claim that process development and design can benefit from improved knowledge-representation schemes and advanced reasoning control strategies. Árva and Csukás (1988) suggest an abstract algebraic representation with fuzzy evaluation. The general development within fuzzy methods and expert system is still going on but only limited reports from process synthesis are noted.

2.5 Process synthesis in perspective.

What are the most important factors for successful energy and/or process optimisation? This question should always be in mind when considering new work in the area of process synthesis. There is no doubt that the following two items are of crucial importance

- In depth knowledge of the process to be optimised
- Knowledge of available synthesis tools and ability to use them efficiently

The level of expertise is highly dependent of the framework in which the analysis takes place. For a large organisation it is possible to include experts in various fields provided the time factor allows it. In minor organisation it is more often the case that the project organisation only consists of a few persons. These few people can either be from the industrial company alone or with consultants. Here it is important to acknowledge the limitation in expertise in each and every field. In that case it is important to make priorities. Process understanding comes first, synthesis knowledge comes next. It is thus important that the available synthesis tools are flexible and easy in use.

Process synthesis may be put in perspective by listing the typical tasks with estimates of expected accuracy of each task.

Task	Expected level of accuracy
Data acquisition/Reconciliation	Within 2 - 10 %
Cost estimates/General cost equations	Within 5 - 30 %
Synthesis	Optimum found within 1-3 % !!!
Validation/ Post synthesis	Major modification due to practical considerations.

It could be argued that optimum in many cases are insensitive of the inaccuracies in the problem formulation. This does, however, require that the inaccuracies are well distributed. For heat exchanger network synthesis e.g. it will be demonstrated (chapter 4.4) that assumption of counter current heat exchange might give unrealistic results when operating with small temperature differences.

If the optima indeed are sensitive to inaccuracies as pointed out above, then it can be concluded that further enhancement in the area of process optimisation should be focused at improving the formulation of the problem instead of improving speed and accuracy of the optimisation routines. There is no sense in achieving optima within few percentages when the accuracy of the problem formulations is significantly inferior.

It is out of these considerations that the present research has evolved. The aim is to enhance the synthesis methods towards including more practical considerations. This is reflected in chapter 6, where a new framework for Heat Exchanger Synthesis is proposed. The aim there is not to provide a new speedy algorithm for the standard literature problems but rather to provide a framework in which important practical issues can be included.

3
PINCH METHOD - STATE OF THE ART

The *Pinch Method* has been strongly promoted by Linnhoff, from the late 70'ies. It is clearly due to his effort that energy integration to day has grown way beyond the academic circles. Today Pinch technology is a well known "tool box" for energy conservation in most of the energy intensive industries and by many energy consulting companies. In education the pinch method is taught in various undergraduate courses all over the world. The success of Pinch Technology is most of all due to its simplicity. From a few day courses, most students or engineers can do energy integration studies with cases that they previously assumed too complicated. The Pinch technology thus stimulates the engineer''s interest in process integration and thereby the understanding of system engineering.Though most of the theory and principles were outlined before Linnhoff entered the scene only limited practical results were achieved and the method was virtually not spread. Hohmann published a PhD thesis in 1971 on heat exchange network design (Hohmann 1971). In one of his main results he merged all hot streams into a single hot stream and all the cold streams into a single cold stream on such a plot, producing what is now known as the process composite curve diagram. Hohmann also noted that the relation between energy cost and capital costs could be determined by this plot. Knowing to day, the value of this insight, it is surprisingly that the work of Hohmann only received little attention.The results obtained in pinch technology plays an important role in this thesis. This is why a thorough review of the Pinch Method is given. Initially the major principles in the pinch method will be introduced. In the remaining part more detailed aspects are discussed.

3.1 Main principles.

The best way to introduce the pinch method is probably by example. The simplest example of a heat exchanger system is to consider a two-stream problem. There is one process stream that needs to be heated and one process stream that needs to be cooled. With the pinch method it is the wish to predict two things.

- Thermodynamic limit of heat recovery
- Economic optimum heat recovery

In this case the initial temperature of the hot stream (stream to be cooled) is 90 °C and the target temperature is 2 °C. The medium is water and the flowrate is 5 kg/s. The cold stream enters with a temperature of 8 °C and a target temperature of 95 °C. The medium is also water and the flow rate is 7 kg/s.

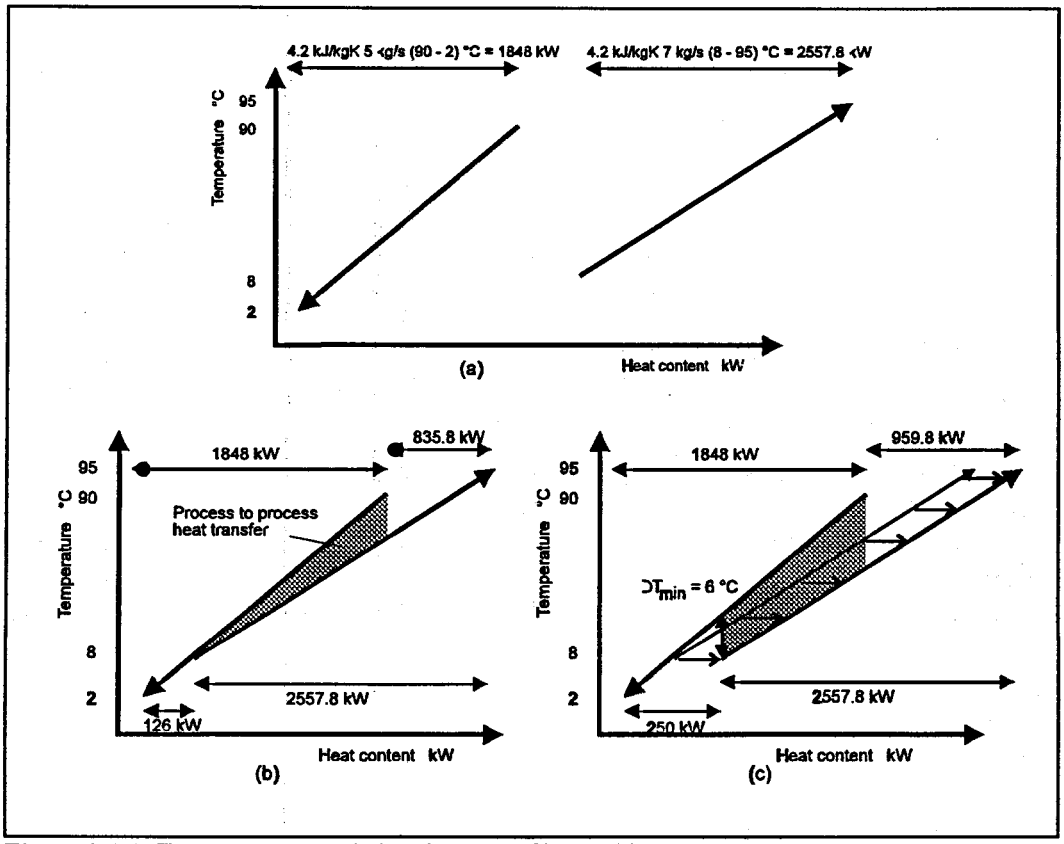


Figure 3.1.1 Temperature - enthalpy diagram of heat exchange process.

In figure 3.1.1a the two streams are plotted in a temperature-heat content diagram. The second law of thermodynamics requires a positive temperature difference when heat is to be transferred from the hot stream to the cold stream. The amount of heat transferred from the hot stream to the cold stream is thus limited by the minimum temperature difference. In figure 3.1.1b the two curves touch each other. The heat recovery is represented by the part where the hot and cold streams are overlapping. The heating and cooling demands are represented by the surplus in each end of the curves. A heat exchanger with a minimum temperature difference will be of infinite size. For practical use there will thus always be considered a certain minimum temperature difference (ΔT_{min}). The minimum energy usage can be found with the specified temperature difference by moving the two curves horizontally away from each other. The individual heat demand and temperatures for the two streams are still the same but another amount of heat recovery is found (figure 3.1.1c).With the simple temperature-heat content diagram it is possible to calculate the heat and cooling demand with any specified ΔT_{min}.As mentioned, the temperature difference influences the size of the heat exchanger. A large temperature difference gives a small heat exchanger while a small temperature difference gives a large heat exchanger. From the temperature-heat diagram it is actually possible to predict the size of the heat exchanger. Therefore it is not only possible to predict the energy use but also the heat exchanger area. The next step is then to predict the capital cost of the heat exchanger equipment and the cost associated with the heating and cooling demand. The cost function is dependent on the heat exchanger size and the energy cost is dependent of the heating and cooling demands. Applying these cost functions the total cost of the heat recovery system can be predicted as a function of ΔT_{min}. Calculating these values

for a range of ΔT_{min} values, it is possible to find the optimum value of ΔT_{min} and thus the economically optimal heat exchanger. This is illustrated in figure 3.1.2, where the present value of expenses is used as objective function. In pinch terminology this is

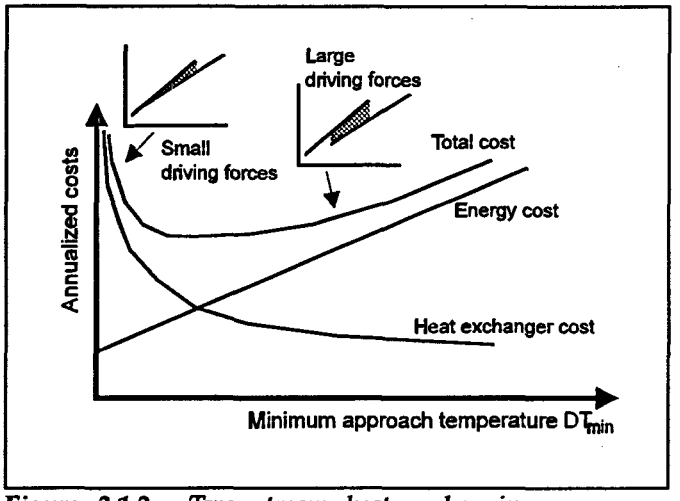


Figure 3.1.2 Two stream heat exchanging process. Energy and capital targeting.

known as supertargeting (Linnhoff and Ahmad This simple example describes the essence of pinch technology - prediction of energy targets and economical targets.The true value of the Pinch Method is, however, that it is possible to enhance the above mentioned approach to include any number of process streams. This is done through combining temperature-heat content curves - into the so-called *Composite Curves* (Linnhoff et al. 1982).Figure 3.1.3 shows two cold streams plotted in a temperature-heat content diagram. The streams are plotted with their respective inlet and target temperatures and their heat demand. The start and target temperatures define boundaries of temperature intervals. In interval 1 only

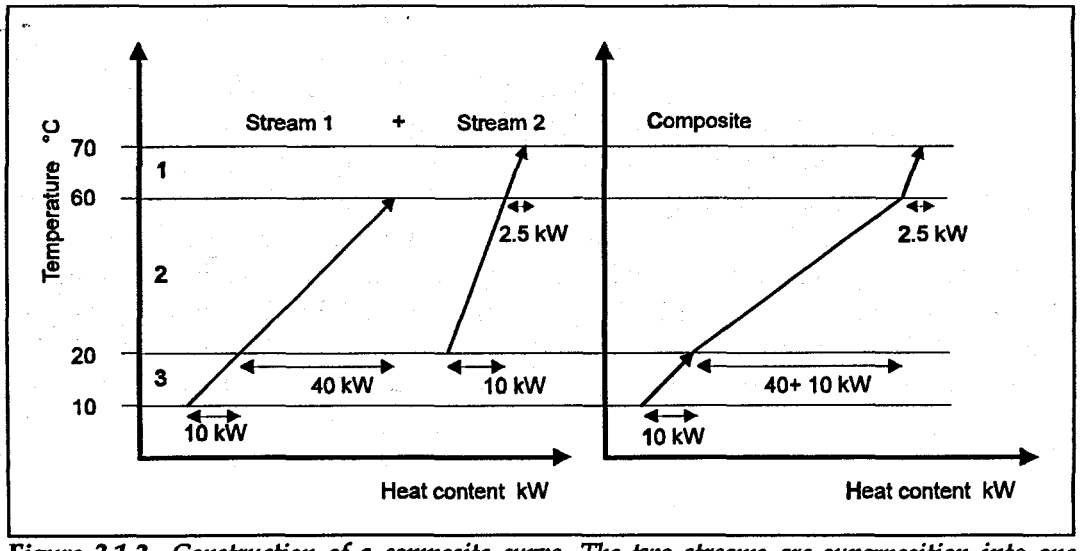


Figure 3.1.3 Construction of a composite curve. The two streams are superposition into one composite curve.

stream 1 exist, in interval 2 both streams exist and in interval 3 only stream 2 exist. These curves are now superposition into one cold composite

The same is done by the hot stream forming a hot composite curve. These curves are plotted in figure 3.1.4. Again the two curves can be move horizontally toward each other until a sufficient minimum temperature approach is

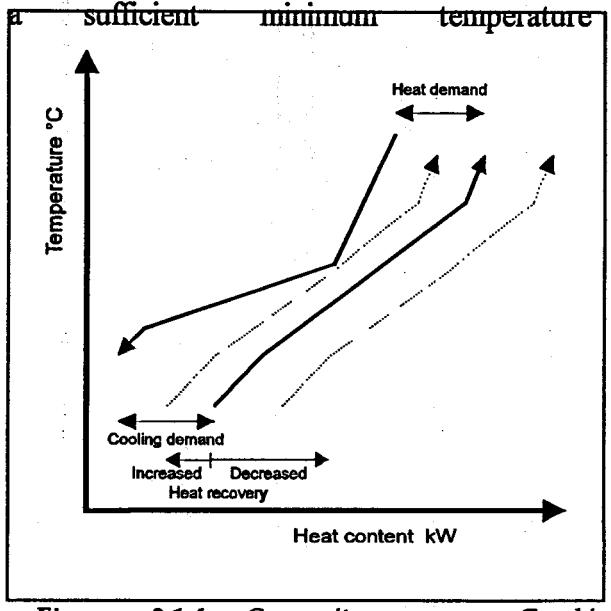


Figure 3.1.4 Composite curves. Graphic determination of minimal heat and cooling demand.

The same arguments for balancing capital and energy cost as with the two-stream problem can be used. The more closely the two curves are placed the more energy is recovered and the more capital cost is needed. Again calculating the total cost for a range of ΔT_{min} makes it possible to determine the optimum heat recovery defined by an optimum value of ΔT_{min}. The primary difference between the two stream example and a multiple stream example is that in the first case the heat recovery system layout is fixed with one heat exchanger. With more than two streams the heat exchanger network is not fixed. In that case several alternative heat exchange network layouts might be possible. A major task is designing a network that fulfils the target calculated with the targeting procedure. Construction of such heat exchanger networks is based on a simple set of rules (see chapter 3.4) and guidelines (chapter 3.10). If the rules are followed, the energy target will always be fulfilled. It is, however, not certain that the capital target is met. The detailed design work to obtain a network that fulfils the capital cost target is much more complicated than just to fulfil the energy target. Actually there is no guaranty that the capital cost target is obtainable. The result from the capital cost targeting is after all only a prediction. Earlier studies e.g. synthesis of nitric acid plants (Hansen and Nielsen, 1991) has shown that networks designed by hand can be within 10 % of the predicted heat exchanger area.

3.2 Energy targets.

Probably the most important feature about the pinch method is the ability to predict the minimum energy demand. This can be done using the graphical approach outlined in the previous chapter. There is however an alternative numerical way of getting the same results. This is done by the "Problem Table Algorithm" (Linnhoff et al. 1982). The approach is based on the second law saying that heat flows from the hot to the

colder body. This principle is utilised in the heat cascade theory where the heat demand or surplus at each temperature interval is cascaded to the temperature interval below by ranging the process streams after temperature. Plotting the process streams on a temperature scale, it is possible to split the temperature scale into

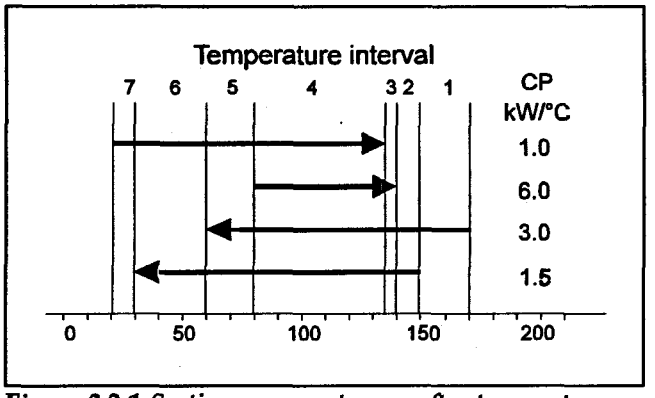


Figure 3.2.1 Sorting process streams after temperatures and establishing temperature intervals.

temperature intervals, each with constant number of process streams (Figure A stream heat capacity flow rate (CP in kW/C) is associated with each process stream.In each temperature interval the heat surplus or deficit is calculated ΔH (kW). In that way the problem table (Linnhoff et al. 1982) can be build.

Interval nr.	1	2	3	4	5	6	7
Temp. diff. $T_i - T_{i+1}$ C	20	10	5	55	20	30	10
ΣCP_{cold} - ΣCP_{hot} kW/°C	-3	-4.5	1.5	2.5	-3.5	-0.5	1
ΔH kW	-60	-45	7.5	137.5	-70	-15	10

A deficit in one interval can be covered by a surplus from the above temperature intervals. If there is not enough surplus in the above intervals external heat must be

Temperature	170	150	140	135	80	60	30	20
Cascaded Heat kW	0	60	105	97.5	-40	30	45	35
Balanced cascade	40	100	145	137.5	0	70	85	75

supplied. The surplus heat is thus cascaded down through the temperature

Since negative heat flow is infeasible there have to be supplied heat. The heat is supplied at a level above the heat deficit point. In the above table the heat is supplied above the highest temperature (inlet to interval 1). The minimum amount of heat

supply (Q_{Hmin}) is achieved when the lowest heat flow equals zero. The point of zero heat flow is the *Pinch point*. The heat out of the last interval (Q_{Cmin}) must be discharged through a cooling system.In the above it is assumed that it''s possible to exchange heat down to zero temperature difference. If a specified ΔT_{min} is to be assured then the real temperatures are shifted into pseudo temperatures in a way that all cold streams seem to be warmer and hot streams seems to be colder. By shifting the temperatures $\Delta T_{min}/2$ respectively the minimum temperature difference will never be less than ΔT_{min} in each pseudo temperature interval.The problem table with the pseudo temperatures can be constructed in the same way as with the real temperatures. This time only a minimum heat and cooling target is found subject to a specified ΔT_{min}.The energy target from the problem table is the same as if using the composite curves. While the composite curves give good visual insights, the problem table is ideal for computational implementation.

3.3 Heat exchange cost targeting.

The area targeting is best illustrated by the composite curves. If the total process to process heat exchange is viewed as one countercurrent heat exchanger, the total heat exchanger area can be calculated by using the log mean temperature approach of each interval (Figure 3.3.1) (Townsend and Linnhoff 1984).

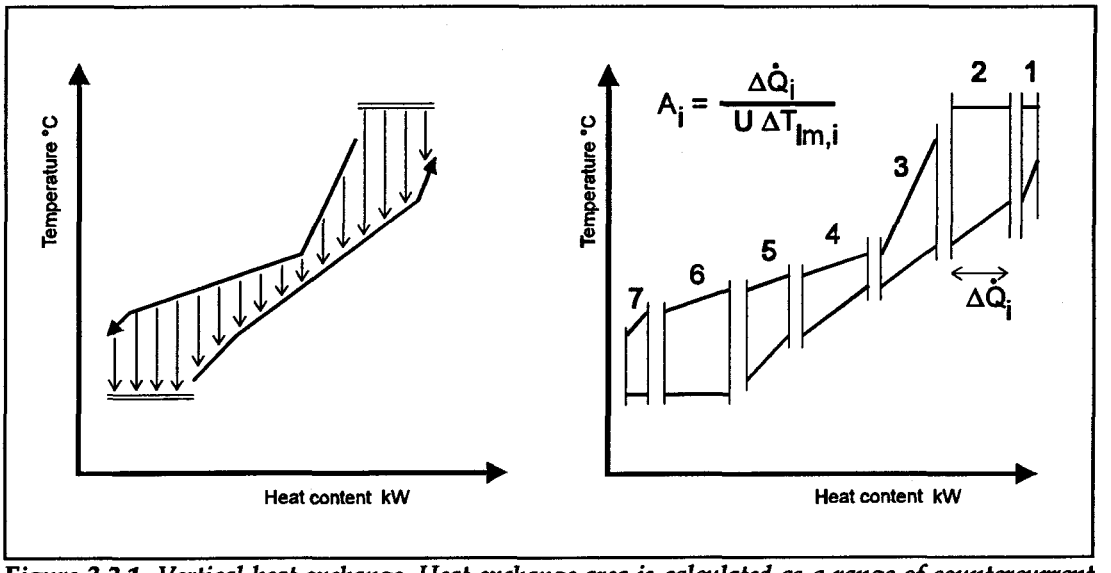


Figure 3.3.1. Vertical heat exchange. Heat exchange area is calculated as a range of countercurrent heat exchangers each with constant properties.

The necessary heat exchange area in each interval can be calculated as

$$A_i = \frac{\Delta \dot{Q}_i}{U \Delta T_{lm,i}} \qquad (3.3.1)$$

where the heat transmission number U is calculated from the heat transfer coefficients h_{hot} and h_{cold}.

$$\frac{1}{U} = \frac{1}{h_{hot}} + \frac{1}{h_{cold}} \qquad (3.3.2)$$

In each interval, each stream (j) thus contribute to the interval area contribution A_i

$$A_{i,j} = \frac{1}{h_j} \cdot \frac{q_{i,j}}{\Delta T_{lm,i}} \qquad (3.3.2b)$$

The log mean temperature difference is constant in each interval. With the assumption of vertical heat transfer the resulting overall heat exchanger network area can be expressed (Townsend and Linnhoff, 1984) as

$$A_{vertical} = \sum^{Intervals,i}\left(\frac{1}{\Delta T_{lm,i}}\right)\sum^{Streams,j}\left(\frac{q_{ij}}{h_j}\right) \qquad (3.3.3)$$

The vertical target is the rigorous minimum area target when the heat transfer coefficients are constant for all hot streams (h_{hot}) and for all cold streams h_{cold}.

Ahmad et al. (1990) stated that the vertical heat transfer model is sufficiently accurate provided the heat transfer coefficients differ by less than one order of magnitude. There are however more elaborate models available in the literature that considers different heat transfer coefficients (Saboo et al. 1986b, Ahmad et al. 1990). These more complex models will shortly be explained in chapter 3.7.

The capital cost for a heat exchanger network is not solely dependent on the heat exchange area but also on the number of heat exchanger units. To predict this number Linnhoff used the Euler General Network Theorem (Linnhoff, 1979).

$$U = N + L - S \qquad (3.3.4)$$

where U is the number of units in a network
N is the number of streams including utilities
L is the number of loops in the network
S is the number of subsets making up the network

For maximum energy recovery (MER) Linnhoff et al. (1982) applied the Euler theorem on each side of the pinch finding the minimum number of units above the pinch and the minimum number of units below the pinch.

$$U_{\min,MER} = U_{\min,above} + U_{\min,below} \qquad (3.3.5)$$

With no loops (L=0) and a single subset (S=1) on both side of the pinch this expression is reduced to

$$U_{\min,MER} = N_{above} + N_{below} - 2 \qquad (3.3.5)$$

To predict the capital cost of a network a general price function of an individual heat exchanger must be assumed. A simple relationship frequently used is

$$Installed\,Cost = C_1 + C_2\ Area^n \qquad (3.3.6)$$

where C_1 is the baseprice
C_2 is the specific area price
n is the area exponent

Assuming equally distributed area on the exchangers the total capital costs can be predicted (Hall et al. 1990) by

$$\textit{Network Capital Cost} = U_{\min,MER}\left(C_1 + C_2\left(\frac{A_{\min}}{U_{\min,MER}}\right)^n\right) \quad (3.3.7)$$

With the total cost estimation it is now possible to predict the total cost (energy and capital) as a function of the minimum approach temperature - ΔT_{min}. This requires that the cost coefficients include the associated costs for installation. If the total cost is calculated for a range of ΔT_{min} values then an optimal ΔT_{min} can be found. This is commonly known as *Supertargeting* (Linnhoff and Ahmad, 1986).

3.4 The Pinch philosophy.

Having introduced the principle elements of the pinch method - Energy and capital targeting - it is now time to look at the general idea, from where the pinch analysis has emerged.

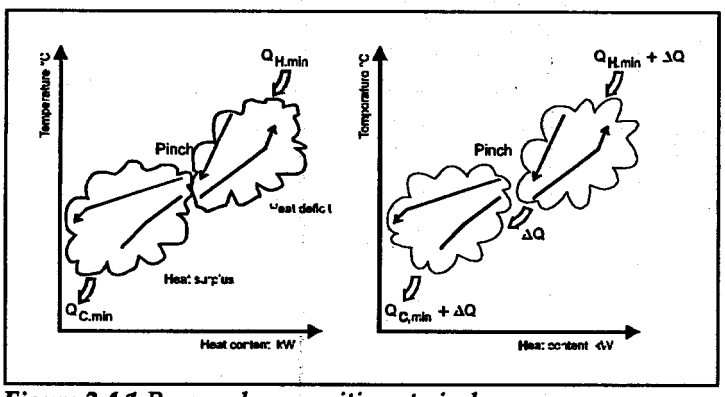


Figure 3.4.1 Process decomposition at pinch.

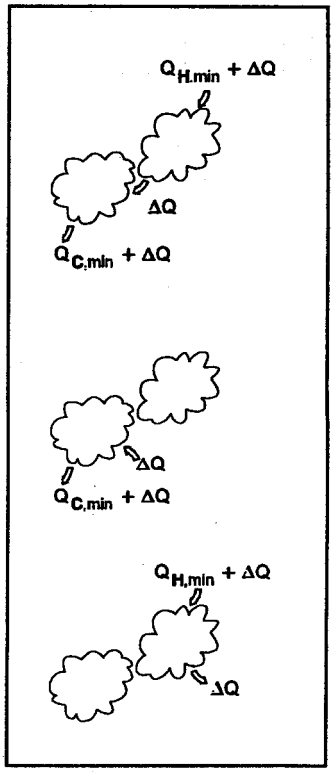


Figure 3.4.2 The pinch principles.

Looking at the process composite curve fig. 3.4.1, it is noticed that the process, thermodynamically, can be decomposed at the pinch. The part above the pinch is in energy balance with the hot utility and the part below the pinch is in energy balance with the cold utility. If more hot utility is supplied, the excess heat must be transferred across the pinch and finally discharged to the cold utility. This was recognised by Linnhoff and co-workers (e.g., Linnhoff et al. 1982, Linnhoff and Vredeveld 1984). They concluded that *Designs meeting the energy target exhibit a zero heat flow across the pinch. Suboptimal designs have a heat flow across the pinch that corresponds to the excess utility consumption both hot and cold* (Linnhoff 1983). It is from this simple but valuable conclusion that most of the subsequent elements of pinch technology has emerged.

Pursuing the conclusion stated above a set of rules can easily be derived (Linnhoff 1982).

- Don't transfer heat across the pinch
- Don't use hot utilities below the pinch
- Don't use cold utilities above the pinch

This set of rules will in the rest of this thesis be referred to as the *Pinch Principle*. These rules are especially important when considering heat engines, heat pumps and process modification that will be discussed in subsequent chapters.

3.5 Utility targeting.

The process-utility interface is best illustrated by the Grand Composite Curve - GCC (Linnhoff et al. 1982). The GCC can be constructed from the Composite Curves - CC or from the problem table.

First the GCC will be derived graphically from the CC. The construction of the GCC is illustrated in Figure 3.5.1. The first step is to shift the temperature by $\Delta T_{min}/2$. The cold composite is shifted $\Delta T_{min}/2$ up and the hot composite ΔT_{min} down. Now the two curves touch each other at the pinch. These shifted composite curves now represent the surplus driving temperature forces assuming a minimum approach temperature ΔT_{min} They also show the amount of heat that is in surplus at each shifted temperature. This amount of heat is plotted against the shifted temperatures forming the GCC.

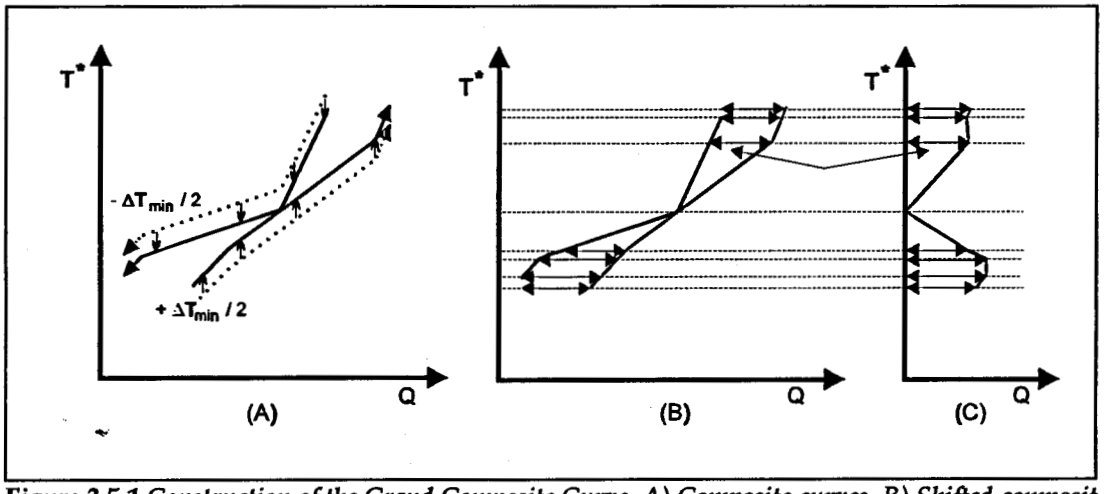


Figure 3.5.1 Construction of the Grand Composite Curve. A) Composite curves. B) Shifted composit curves. C) Surplus heat at each shifted temperature.

To construct the GCC from the Problem Table - chapter 3.2 is even simpler. In the problem table the surplus heat out from each shifted temperature level is calculated directly. This procedure gives an alternative easy numerical method to construct the GCC.

The information provided by the GCC is mainly of what levels heat is to be supplied or removed. It is important to notice that the GCC is constructed under the assumption of perfect process to process heat transfer. If the Heat Exchanger Network is not optimal then the GCC only represents heat load under ideal conditions.

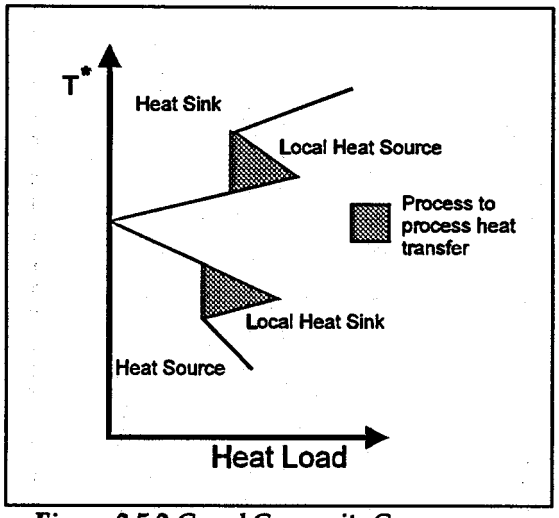


Figure 3.5.2 Grand Composite Curve.

The part of the GCC above the pinch represents the overall *Heat Sink* and the part below the *Heat Source* (Townsend and Linnhoff 1983b). There can however be local heat sources above the pinch and local heat sinks below the pinch - Figure 3.5.2. For these local heat sinks and sources the process to process heat transfer takes care of the energy requirements. It should however be noticed that these local heat sinks and sources represent a surplus temperature difference and thus a thermodynamic inefficiency according to the second law of thermodynamics. This aspect will be further discussed in chapter 3.6.

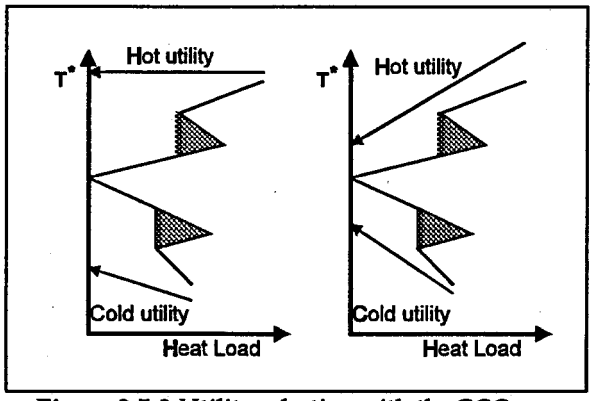


Figure 3.5.3 Utility selection with the GCC.

The primary use of the GCC is to select temperature levels for utilities. The simplest case is when only one cold and one hot utility are to be used. In Figure 3.5.3 two examples of utility placement are shown. The hot utility must be fully above the pinch and the cold utility fully below the pinch according to the pinch principle.

In many cases, however, it is beneficial to use several hot and cold utilities utilising the differences in energy costs. An example of multiple utilities is shown in Figure 3.5.4 where two different levels of steam and two different levels of cooling are supplied. The feasibility of a utility selection is easily identified using the GCC.

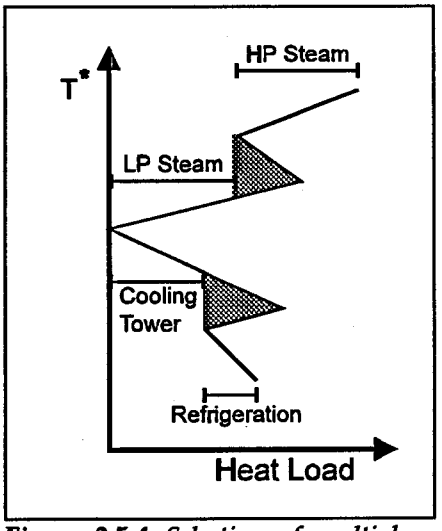


Figure 3.5.4 Selection of multiple utilities.

When the utilities are selected, new modified Composite Curves and Grand Composite Curves can be constructed. These derived curves are called Balanced Composite Curves - BCC (Parker 1989) and Balanced Grand Composite Curves - BGCC (Hall 1989).

The BCC is constructed by translating the utilities into streams. The new CC curve is then redrawn, incorporating the new streams - Figure 3.5.5.

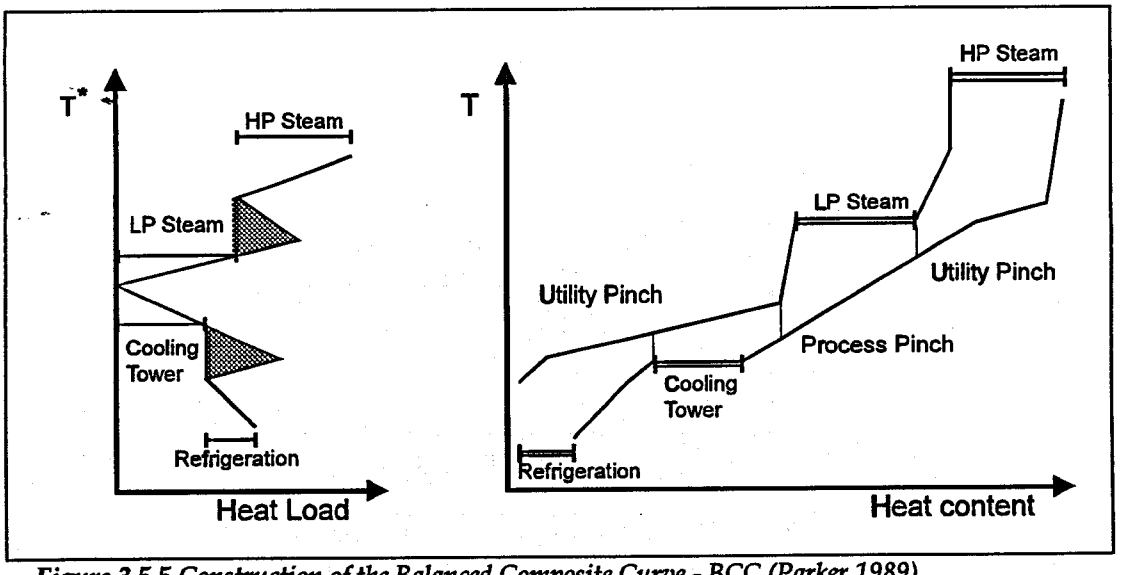


Figure 3.5.5 Construction of the Balanced Composite Curve - BCC (Parker 1989).

The BCC represents the driving forces considering the utility selection. It is the BCC that is used for calculating the overall heat exchange area demand. When using the BCC no energy is supplied or removed externally.

Hall (1989) introduced the Utility Grand Composite Curve - UGCC, that represents the utilities matching a given process GCC. Construction of the UGCC is similar to the construction of the process GCC. In Figure 3.5.6 (reconstructed from Hall et al. 1992) it is shown how the UGCC is constructed from the balanced utility streams.

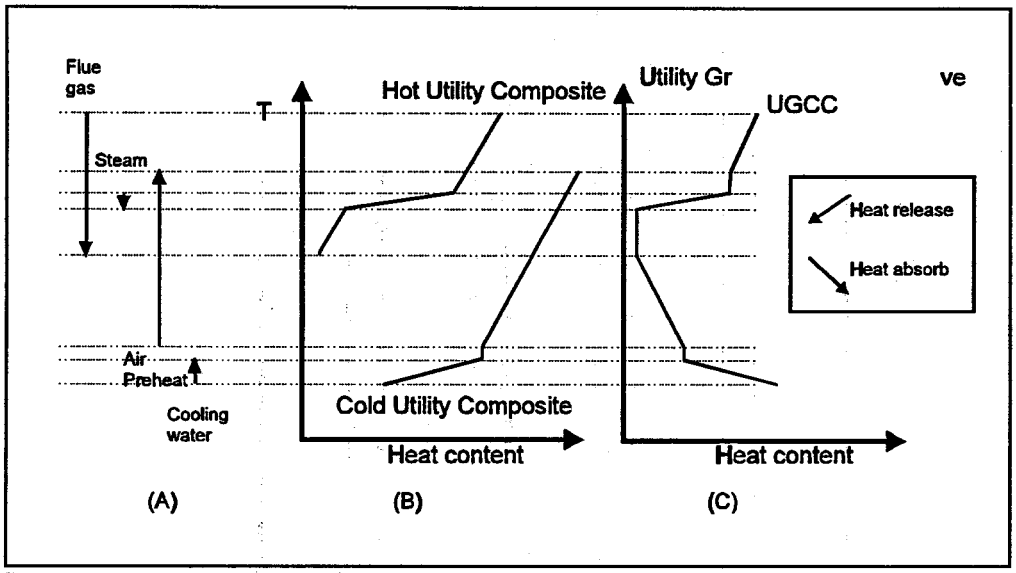


Figure 3.5.6 Construction of the Utility Grand Composite Curve - UGCC. A) Utility streams. B) Utility composite curves. C) Utility Grand Composite Curve (after Hall 1989).

The UGCC is heat releasing when the slope is positive and heat absorbing when the slope is negative. The UGCC shows the net heating and cooling duties that the selected utilities can supply. Combining the UGCC with the process GCC gives the so called Balanced Grand Composite Curve - BGCC - Figure 3.5.7 (Hall 1989).

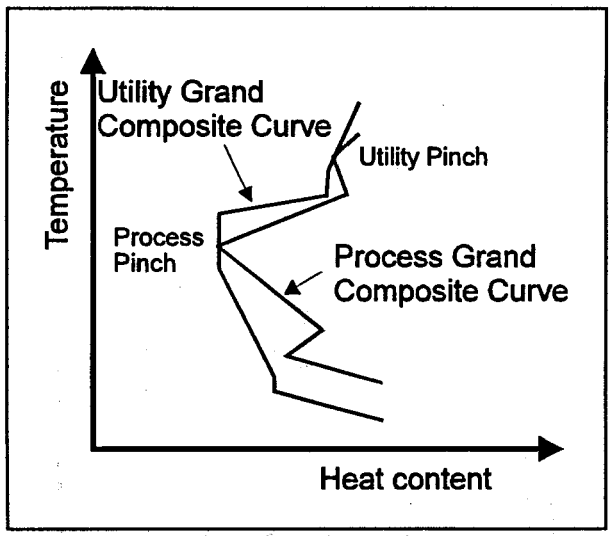


Figure 3.5.7 The Balanced Grand Composite Curve is the combination of the Process GCC and the Utility GCC (After Hall 1989).

Combining the two GCC's might cause additional pinch points. These are normally noted *Utility Pinches* (Hall et al. 1992). While the process pinches are caused by the process concept the utility pinches are caused by the utility selection. This implies that it should be easier to control the utility pinches than the process pinches. In practice this means that if the process pinch is to be beaten then the process has to be changed. If on the other hand the utility pinches is to be beaten, then the utility system has to be changed. The latter normally allow the highest degree of freedom.

While the energy - capital trade off for single hot and single cold utilities is well described (e.g. Linnhoff and Ahmad 1989), the energy - capital trade off for multiple utility system is still rather unexploited. Currently two approaches have been suggested - one based on the Balanced Grand Composite Curves - BGCC (Hall 1989) and the other based on the Balanced Composite Curves - BCC and the supertargeting concept (Parker 1989).

Both general approaches will be shortly outlined by using the examples from Hall et al. 1992.

3.5.1 Using BGCC (Hall 1989).

In this example a process is considered with a process GCC as shown in Figure 3.5.8. The utility system consists of FlueGas (FG), Steam (ST), Air Preheat (AP) and Cooling Water (CW). The resulting UGCC is drawn together with the process GCC (Figure 3.5.8). Initially arbitrary loads and air temperature are used to draw the first UGCC. The process GCC and initial UGCC can now be used to form the first Balanced GCC (this is actually Figure 3.5.8).

It is important at this stage to understand the degrees of freedom for the utility system. For this system with fixed fuel to air ratio the important utility parameters are fuel flow, flue gas exit temperature, air preheat temperature, steam flow and cooling water flow. The number of freedom for this utility system is thus 4 (5 - 1 the system must balance)

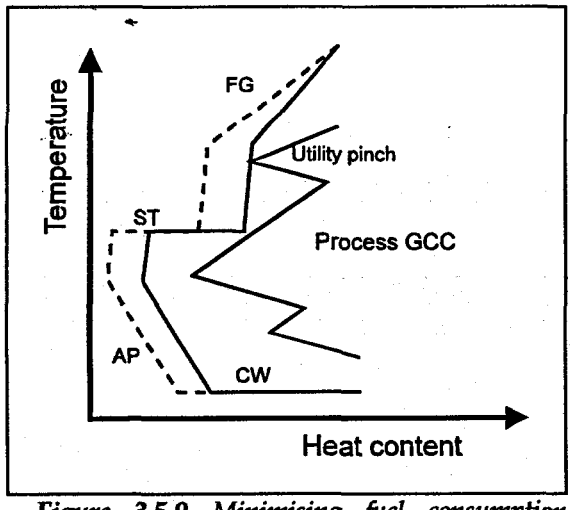


Figure 3.5.9 Minimising fuel consumption (FG).

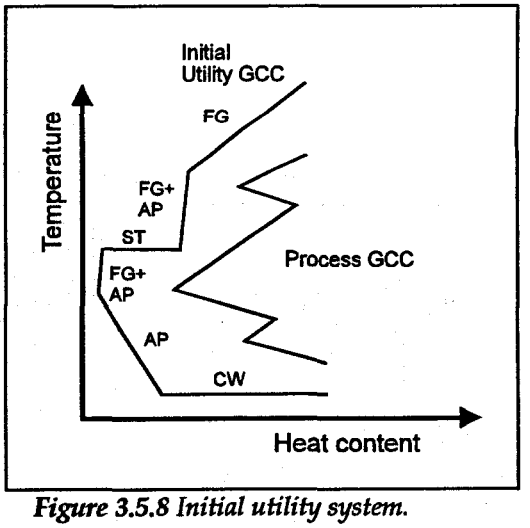


Figure 3.5.8 Initial utility system.

By using the BGCC it is easy to see whether the selected heat load gives a feasible solution or not. The objective is to minimise energy costs. A way to do this is to minimise or close the gaps between the process GCC and the UGCC. In the initial BGCC (Figure 3.5.8) there is no utility pinches (touches between the two GCC's). Hall et al. (1992) now suggests considering one utility at a time, starting with the most expensive. In this case fuel is assumed to be the most expensive so the first step

is to reduce the fuel first. A change in fuel will only result in a change in slope of the fluegas and in air preheat. The limit of flue gas reduction is met when the two curves touch each other. The resulting pinch point is called a utility pinch. In Figure 3.5.9 the new modified BGCC is shown. It is noticed that the CW utility has decreased accordingly.

The next option is to reduce the air preheat temperature. This will result in a new flue gas temperature but the slope will be constant. Again the reduction is limited by the process GCC (Figure 3.5.10). The final step is to consider the two remaining utilities - Steam and cooling water. To fulfil the energy balance these two utilities must be reduced simultaneously. They can be reduced until a new utility pinch occurs (Figure 3.5.11).

Using the Balanced Grand Composite Curve gives a good graphical representation of the utility selection problem. This representation is well suited for high level engineering were use can be made of the thermodynamic principles.

The approach is, however, based on minimising the energy cost on the assumption that an optimum overall ΔT_{min} is known. This subsequently leads to the assumption that each utility is optimally determined when they cause a new pinch (utility pinches). The approach does not account for the energy - capital cost trade off for each individual

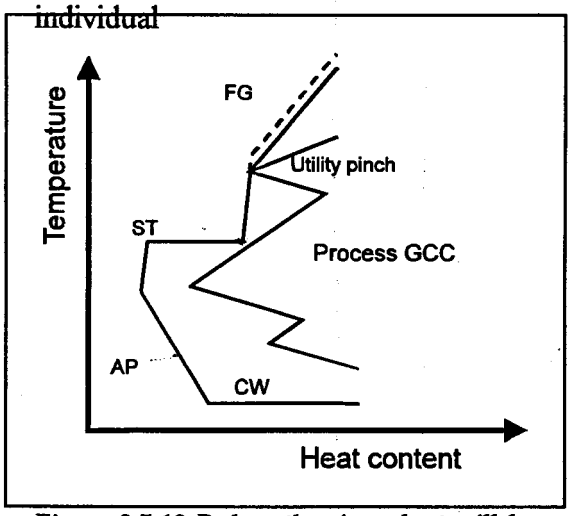


Figure 3.5.10 Reduce the air preheat will lower the flue gas temperature.

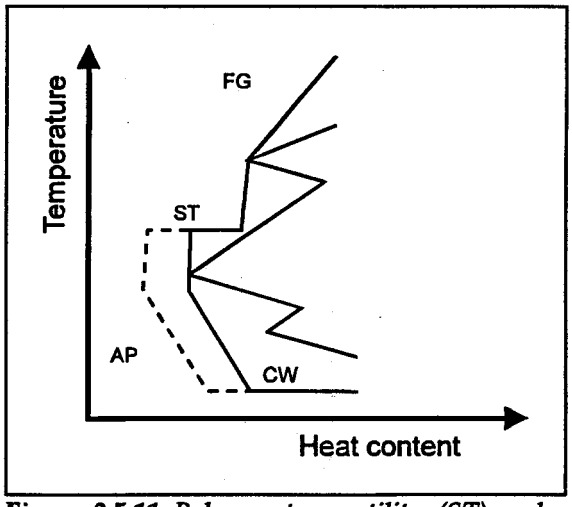


Figure 3.5.11 Balance steam utility (ST) and cold water utility (CW).

3.5.2 Using BCC

Parker (1989) proposes another approach to the multiple utility selection based on the Balanced Composite Curves. As mentioned earlier in this chapter the BCC gives a picture of the driving forces for the integrated utilities. They can thus be used to calculate the total heat transfer area for the process including the selected utilities.

For the single hot/cold utility problem the BCC can be used to trade off capital costs for energy costs. For the multiple utility problem however there are more degrees of freedom (DOF). For the general trade off there is N-1 DOF, where N is the number of utilities (Parker 1989).

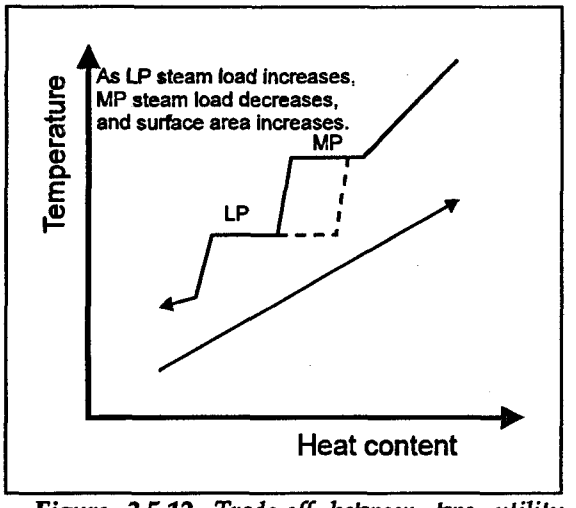


Figure 3.5.12 Trade-off between two utility levels (Parker 1989).

In Figure 3.5.12 the effect of trading of two utility levels on energy and capital costs is shown. If LP steam is increased, the requirement for MP steam will be decreased which lead to lower energy cost. On the other hand the heat exchanger cost will increase due to the decrease in driving forces. Thus energy cost can be traded of for capital cost finding the optimum distribution of LP and MP steam. In this case a fixed overall energy consumption is assumed. If there for the same problem is considered all utility levels a more complex multidimensional trade off is faced. Parker points out that the key to the global trade off is an understanding of these individual trade off's. To solve this problem he suggests a sequential approach where the utilities are traded off individually starting from the pinch.

The approach suggested by Parker allows for systematic trade off of utility levels. The major draw back for this approach, is that each individual trade off results in a local optimum, that is not necessarily a part of the global optimum. It is however not clear how much this affects the practical use of the above approach.

3.6 Heat engines.

For integrating heat engines and heat pumps into the process two elements of the pinch method is important.

- Pinch principle
- Grand Composite Curve

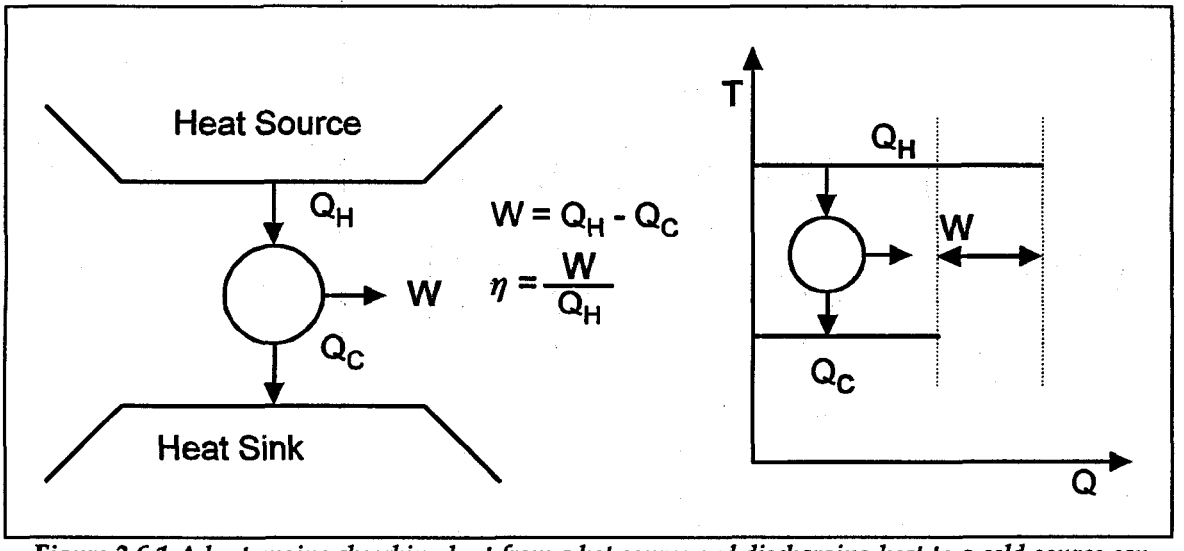


Figure 3.6.1 A heat engine absorbing heat from a hot source and discharging heat to a cold source can be represented in a T-Q diagram.

A heat engine can, from a thermodynamic point of view, be treated as a device that absorbs heat from a heat source and rejects the heat to a heat sink. The work from the device W is the difference between the absorbed heat Q_H and the heat rejected Q_C. In Figure 3.6.1 the heat engine is plotted in a temperature - enthalpy diagram assuming constant temperature for the heat sink and source.

The first law thermal efficiency η of a heat engine is normally given as the ratio between produced power W and the absorbed heat Q_H.

$$\eta = \frac{W}{Q_H} \tag{3.6.1}$$

If the heat engine is integrated with the process an alternative efficiency will be considered based on system performance. The new integrated/marginal efficiency η_i is calculated as the ratio between the power output W and the increased energy demand for the process including the heat engine ΔQ_H.

$$\eta_i = \frac{W}{\Delta Q_H} \tag{3.6.2}$$

In Figure 3.6.2 different heat engine integration schemes are considered. Figure 3.6.2a shows the heat engine (represented in T-Q diagram) and the GCC for the process in which the engine is to be integrated. In (b) the heat engine is integrated in a way that the heat rejection from the heat engine can be utilised by the process. The engine is integrated fully above the pinch. From the figure it is noticed that the additional heat demand corresponds to the power output. The resulting power output is thus produced with a marginal efficiency $\eta_i = 1$. The cooling demand is not affected by the heat engine integration. In (c) the engine is placed in a way that all heat to the engine is absorbed from the process. The heat from the engine is in this case rejected to the cold utility system. The engine is in this case placed fully below the pinch. There is no need for additional heat that results in an integrated efficiency that is infinite (W/0). Since energy is net removed below the pinch a reduction in cooling requirements also results. Finally in (d) the heat engine is placed across the pinch with the heat source above the pinch and the heat sink below the pinch. The result is that there is a one to one correspondence between heat to the engine and the additional heat to the total system. The same goes for the cooling part. Using this integration scheme we will end up with an integrated efficiency that is identical with the non-integrated case (a).

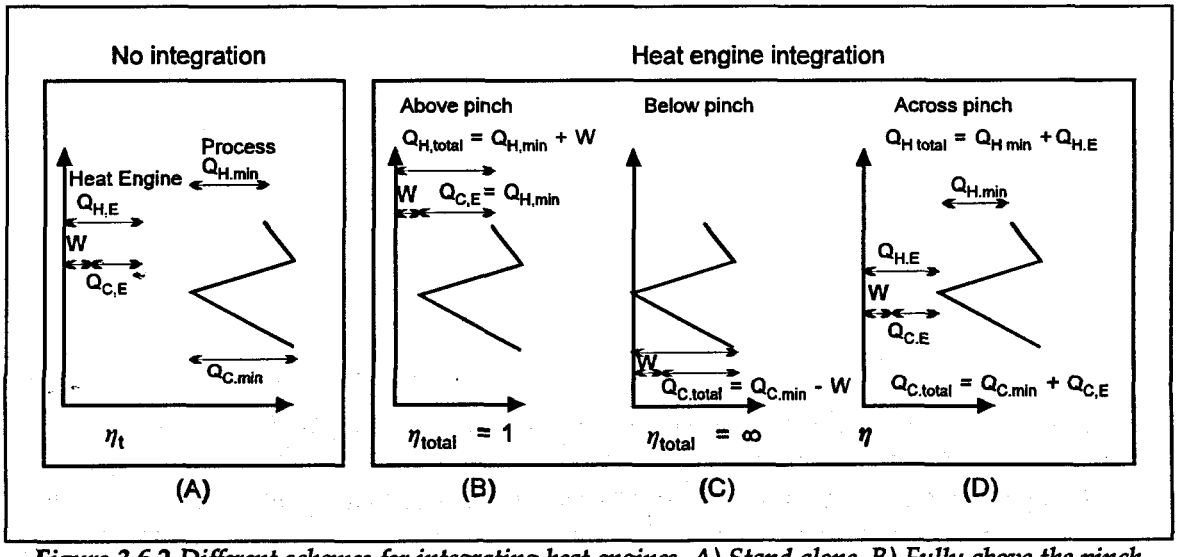


Figure 3.6.2 Different schemes for integrating heat engines. A) Stand alone. B) Fully above the pinch. C) Fully below the pinch. D) Across the pinch.

This effect could actually have been predicted using the pinch principles. In case (b) heat is supplied above the pinch which is in accordance to the pinch principles. In case (c) heat is removed below the pinch which is also in accordance with the principles. In the last case heat is removed above the pinch and released below - both against the pinch principles.

It is then possible to put forward the following guidelines based on the pinch principles applied to heat engines (Townsend and Linnhoff, 1983)

Place heat engines fully above or fully below the pinch
Do not place the heat engine across the pinch

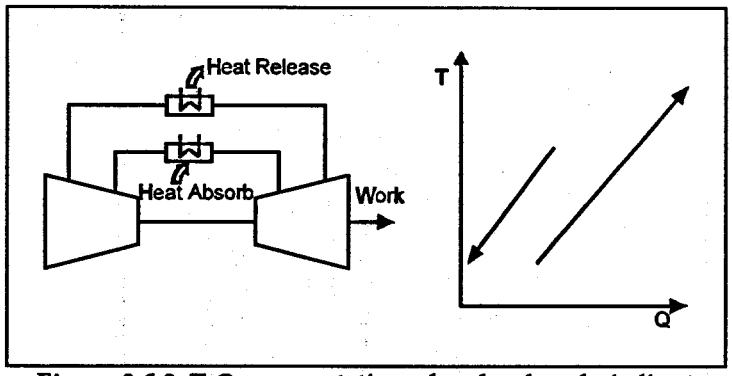


Figure 3.6.3 T-Q representation of a closed cycle indirect fired gas turbine.

The constant temperature heat engine used in Figure 3.6.2 is a reasonable conceptual model for a steam turbine operating between two steam levels. To show that the above rules also apply for other heat engines an indirect gas turbine cycle is considered (fig. 3.6.3). The gas turbine can be represented by the turbine inlet and outlet streams.

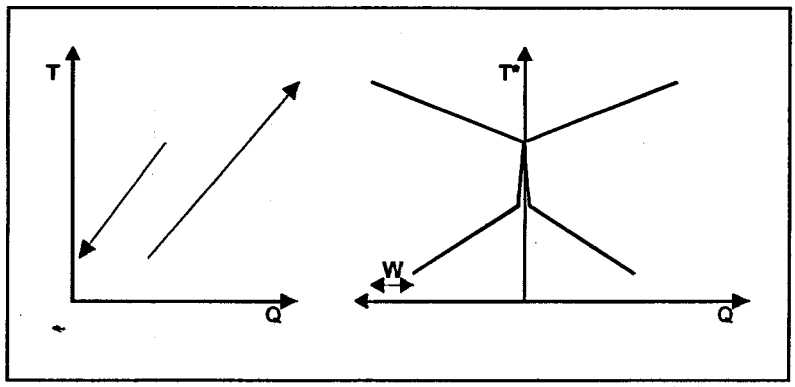


Figure 3.6.4 Heat Engine Grand Composite Curve (HEGCC) for closed cycle gas turbine.

At this stage a new concept will be introduced - a Heat Engine Grand Composite Curve (HEGCC). It is constructed similarly to the Utility Grand Composite Curve. To build the HEGCC simply construct a normal grand composite curve from the streams involved in the heat engine. Then mirror the GCC through the temperature axis (Figure 3.6.4).

The new HEGCC can now be placed together with the process GCC. Investigating different integration schemes (Figure 3.6.5) the same results are obtained with a closed cycle Brayton process as for the constant temperature model. It is worth to notice that in the case of a closed cycle heat engine the gap on the HEGCC represents the gross power output. For an open cycle this is can generally not be expected.

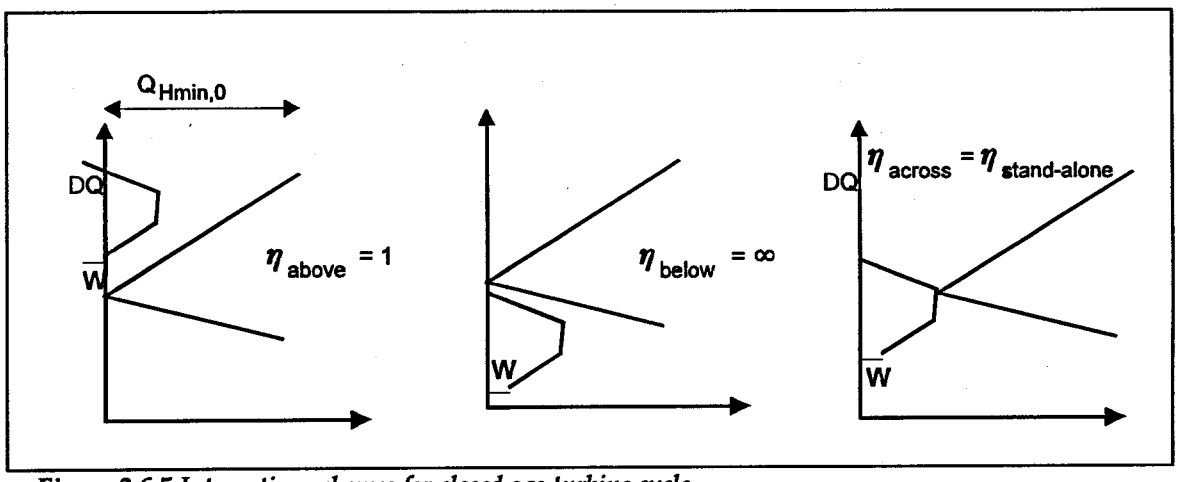


Figure 3.6.5 Integration schemes for closed gas turbine cycle.

It is also possible to construct a HEGCC for a combined heat engine. A combined engine commonly met is the combined cycle consisting of a gas turbine and a steam turbine. Construction of a HECC for a combined cycle is shown in Figure 3.6.6 (a).

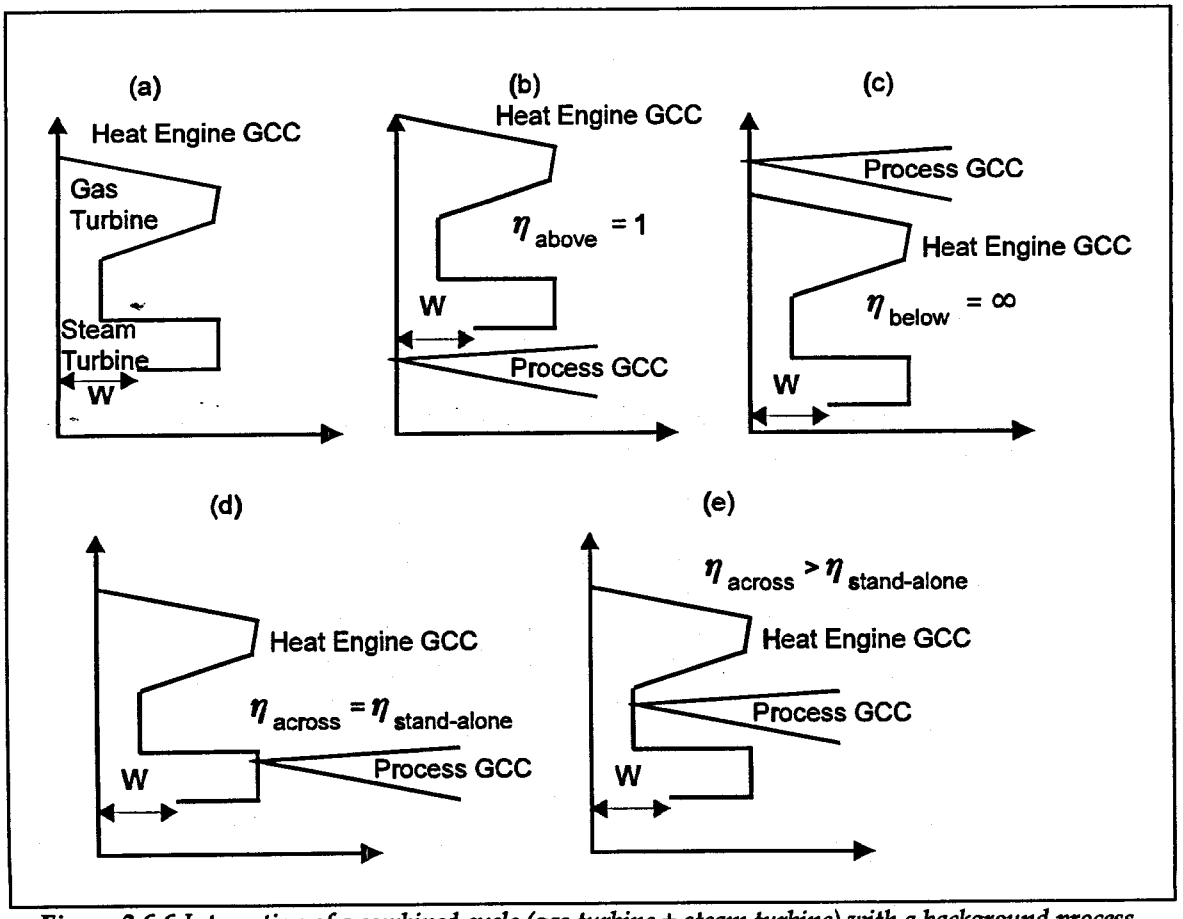


Figure 3.6.6 Integration of a combined cycle (gas turbine + steam turbine) with a background process.

The HECC is combined with the process GCC - Figure 3.6.6 (b). The results from the combine cycle are comparable with the results from the individual cycles. A marginal efficiency of 1 is obtained if the HECC is placed fully above the pinch and an infinite marginal efficiency if it is placed fully below the pinch. Now placing the combined

engine across the pinch some interesting results occur. If the HECC is placed as in 3.6.6 (d) the usual result occurs: no gain in marginal efficiency by integrating the cycle. But if the HECC instead is matched the GCC as shown in 3.6.6.e a considerable increase in marginal efficiency is achieved. It will actually be better to integrate the engine across the pinch than to integrate it fully above.

What is the reason for this apparently surprising result?
When the heat engine placement guidelines were derived from the pinch principle it was indirectly assumed that there was no internal heat transfer in the heat engine. In the combined cycle there actually is a heat transfer over a finite temperature difference. This results in a second law inefficiency. By exploiting this exergy source by matching the process GCC it is possible to increase the overall marginal efficiency. What actually happens when matching the HECC and GCC is that heat transfer from above the pinch to below the pinch is prevented. The combined cycle has in this case been decomposed.

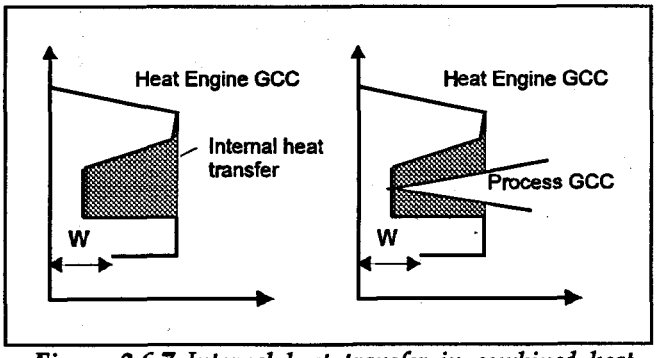


Figure 3.6.7 Internal heat transfer in combined heat engines.

Looking at the HECC (Figure 3.6.7) a heat transfer region is identified - Utility to utility transfer - which will be defined as a HECC pocket. For HECC with no pockets the general guideline is valid while for HECC featuring pockets, these pockets must be examined for exploitation.

3.7 Advanced capital cost targeting.

As mentioned in chapter 3.2, the basic heat exchanger network area targeting equation 3.3.3 is derived under assumptions of: uniform heat transfer coefficients, one common cost law for all exchangers and countercurrent heat transfer. In this chapter methods for handling more complex situations will be shortly discussed.

For non uniform heat transfer coefficient that does not differ significantly, say less than one order of magnitude, it is generally accepted that the basic area target model (eq. 3.3.3) is sufficient. In the case of significantly different heat transfer coefficients Saboo et al. (1986) suggested an improved area target model. The model is based on setting up many small temperature intervals (TI) and solving the following LP problem

$$A_{\min} = \min \sum^{hot\ stream,i} \sum^{cold\ stream,j} \sum^{hot\ TI,k} \sum^{Cold\ TI,l \in S_{lk}} \left[q_{ik,jl} \frac{\left(\frac{1}{h_i} + \frac{1}{h_j}\right)}{\Delta T_{lmik,jl}} \right] \qquad (3.7.1)$$

subject to

Energy balances on hot streams

$$\sum^{Streams,j} \sum^{TI,k \in S_{lk}} q_{ik,jl} = Q_{ik} \qquad (3.7.1)$$

and cold streams

$$\sum^{Streams,i} \sum^{TI,k \in S_{lk}} q_{ik,jl} = Q_{jl} \qquad (3.7.2)$$

where

A_{min}	is the target heat exchanger area
$qk_{,jl}$	is the heat transferred from hot stream *i* in TI k to cold stream j in TI l,
Q_{ik}	is the total heat duty for stream i in TI,
h_i	is the film heat transfer coefficient of stream i,
$\Delta T_{lm\ ik,jl}$	is the log mean temperature difference for an exchanger between stream i in TI k and stream j in TI l,
S_{lk}	is the set of cold intervals for which $\Delta T_{ln\ ik,jl} > 0$
S_{kl}	is the set of hot intervals k for which $\Delta T_{ln\ ik,jl} > 0$

Saboo et al. (1986) noted that the main drawback of the procedure is that the proper division of temperature intervals is not established. They initially started dividing the

temperature range into intervals based on kinks on the composite curves. They then successively make the TI smaller until A_{min} converges or the problem becomes to large.

Ahmad et al. (1990) examined an example where the heat transfer coefficients varied from 0.1 to 5 kW/m²°C. They then calculate the total area target using different approaches. Comparing the result from the LP model and the simple vertical heat transfer model shows a deviation of 29 %.

For problems where the cost laws are not uniform Hall et al. (1990) derive a simple extension to the basic area equation.

$$A^*_{\min} = \sum^{intervals,i} \sum^{streams,j} \left(\frac{q}{\Delta T_{\ln}}\right)_i \left(\frac{1}{\phi h}\right)_j \tag{3.7.3}$$

where the weighting factor ϕ is derived from the heat exchanger cost laws. Assuming one stream that needs special heat exchanger material the special cost law can be written

$$Installedcost = C_1^* + C_2^* \, Area^{n^*} \tag{3.7.4}$$

and for the reference exchanger

$$Installedcost = C_1 + C_2 \, Area^n \tag{3.7.5}$$

By assuming fixed baseprice ($C_1 = C^*_1$) and fixed area exponent ($n = n^*$) Hall et al. derives the expression for the ϕ-factor

$$\phi = \left(\frac{C_2}{C^*_2}\right)^{1/n} \tag{3.7.6}$$

Equation 3.7.7 is then used in (3.7.4) when the heat transfer does not differ significantly. When the weighted heat transfer coefficients h do differs significantly, Hall et al. suggest to use the linear programming method described by Saboo et al (1986).

Another aspect that will be discussed is the use of non-countercurrent heat exchangers. Heat exchangers in most chemical process plants are dominated by tube and shell heat exchangers, which does not feature full countercurrent heat transfer. The most dominant method for accounting for non countercurrent behaviour is to apply a correction factor F_T to the heat transfer equation (Perry, 1984):

$$Q = UA\Delta T_{lm} F_T \tag{3.7.7}$$

The correction factor is usually expressed in terms of thermal efficiency P and the capacity flow ratio R (Ahmad et al. 1990):

$$P = \frac{(T_{Hi} - T_{Ho})}{(T_{Hi} - T_{Ci})} \tag{3.7.8}$$

$$R = \frac{CP_H}{CP_C} = \frac{(T_{Co} - T_{Ci})}{(T_{Hi} - T_{Ho})} \tag{3.7.9}$$

For a multipass 1-2 exchanger (N shells in series) the correction factor can be derived (Ahmad 1985)

$$F_T = \frac{\sqrt{R^2+1}*\ln\left[\frac{(1-y)}{(1-RY)}\right]}{(R-1)*\ln\left[\frac{2-Y(R+1-\sqrt{R^2+1})}{2-Y(R+1+\sqrt{R^2+1})}\right]} \tag{3.7.10}$$

where

$$Y = \frac{1-\left(\frac{1-RP}{1-P}\right)^{\frac{1}{N}}}{R-\left(\frac{1-RP}{1-P}\right)^{\frac{1}{N}}} \tag{3.7.11}$$

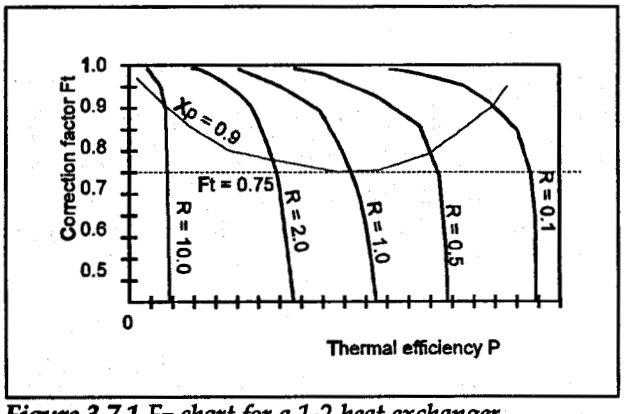


Figure 3.7.1 F_T *chart for a 1-2 heat exchanger.*

In Figure 3.7.1 a F_T chart for a 1-2 exchanger equivalent to equation 3.7.11 and 3.7.12 is showed. For maximum stability and flexibility it is advisable to design heat exchangers with a specified minimum slope (dF_T/dP). Ahmad et al. (1988) use a simple criteria for designing flexible heat exchangers based on keeping an

equidistance to the infinite slope (dF_T/dP), by finding the $P=P_{max}$ for which the slope is infinite.

$$P_{max} = \frac{2}{\left(R + 1 + \sqrt{R^2 + 1}\right)} \tag{3.7.12}$$

For practical design they suggested an equidistance $X_P = 0.9$.

$$P = X_P \, P_{max}, \quad 0 < X_P < 1 \tag{3.7.13}$$

The line for constant $X_P = 0.9$ is shown in Figure 3.7.1.

Ahmad (1985) has derived an analytical expression for calculating the number of shells N based on equations 3.7.9 - 3.7.14 for a specified X_p

$$N = \frac{\ln\left[\frac{1 - RP}{1 - P}\right]}{\ln[Z]} \tag{3.7.14}$$

where

$$Z = \frac{R + 1\sqrt{R^2 + 1} - 2 X_p R}{R + 1\sqrt{R^2 + 1} - 2 X_p} \tag{3.7.15}$$

This goes for one heat exchanger. For heat exchanger network Ahmad and Smith calculates the total number of shells by dividing the process composite Curve into enthalpy intervals and calculate the number of shells (non integer) necessary in each interval.

The non-integer number of shells is rounded up each side of the pinch, estimating the number of shells above pinch and below pinch. Ahmad and Smith (1987) further showed that it is possible to predict the minimum tube-shell area $A_{min,1\text{-}2}$ from the composite curve in a similar way as for the counter-current area. Further a cost target based on number of shells can be derived similar to the simple cost targeting - equation 3.3.7.

$$Capitalcost = C_1 \, U_{min} + C_2 \, N_{shells} \left(\frac{A_{min,1\text{-}2}}{N_{shells}}\right)^n \tag{3.7.16}$$

where

C_1	is the heat exchanger base cost
C_2	is the heat exchanger area cost factor
n	is the area exponent

Even with advanced targeting methods, some limitation must be expected. First of all the assumption of equal heat transfer area distribution between all the exchangers, which is used in all cost targeting methods, gives a notorious uncertainty. An possible refinement is to apply a distribution model (f.x. Gauss) for distributing the heat exchange area among the units.

The importance of targeting must, however, not be overemphasised. It is important to remember that targeting primarily is needed to get an estimate of the total cost for supplying a given set of process streams. It is therefore in most cases enough with a rough estimation. This is especial the case if the detailed network design optimisation is able to account for these conditions (non-uniform heat transfer, cost laws etc.).

The choice of cost targeting model is dependent on the purpose of the analysis and also software availability. The latter is quite important since the detailed targeting methods are not available for most practisers.

3.8 Appropriate placement of unit operations.

In chapter 3.6 it was showed how the Pinch Principle could be used in terms of integrating a heat engine. In this chapter the more general approach for integrating unit operations will be outlined. The pinch terminology normally used for this approach is called appropriate placement.

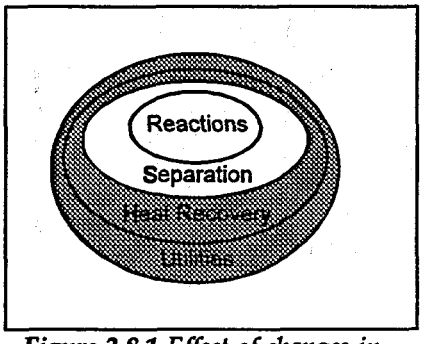


***Figure 3.8.1** Effect of changes in the core process can be predicted using pinch technology.*

At this point only the two outer layers of the onion diagram has been discussed - Figure 3.8.1. It is shown that it is possible to set targets for energy recovery and utility consumption. So far all process streams has been assumed constant. In many cases, however, it can be very beneficial to look into the core process (reaction path and separation path). Knowing that it is possible to calculate energy, capital and co-generation targets from a given set of process streams it is straight forward to propose a strategy for evaluation of process changes.

1. Use initial process core parameters.
2. Get process streams.
3. Calculate targets.
4. Change process core parameters.
5. Calculate new targets - evaluate changes.
6. Repeat 4-5.

This approach is straight forward and can be carried out quickly if a few different process alternatives are considered. There is, however, guidelines developed based on the Pinch Principle that makes use of the thermodynamic insight provided by the pinch analysis. There are specific guidelines for process units as well as general guidelines.

The general guideline, which is called the Plus/Minus Principle, is saying that any process changes which:

1. Increases the total hot stream heat duty above the pinch.
2. Decreases the total cold stream heat duty above the pinch
3. Decreases the total hot stream heat duty below the pinch
4. Increases the total cold stream heat duty below the pinch.

will bring about a decrease in utility requirement (Smith and Linnhoff, 1988).

Moving a hot stream from below the pinch to above the pinch will therefore be especially beneficial since it will contribute to a decrease in heating demand as well in cooling demand. The same goes for shifting a cold stream from above the pinch to below the pinch.

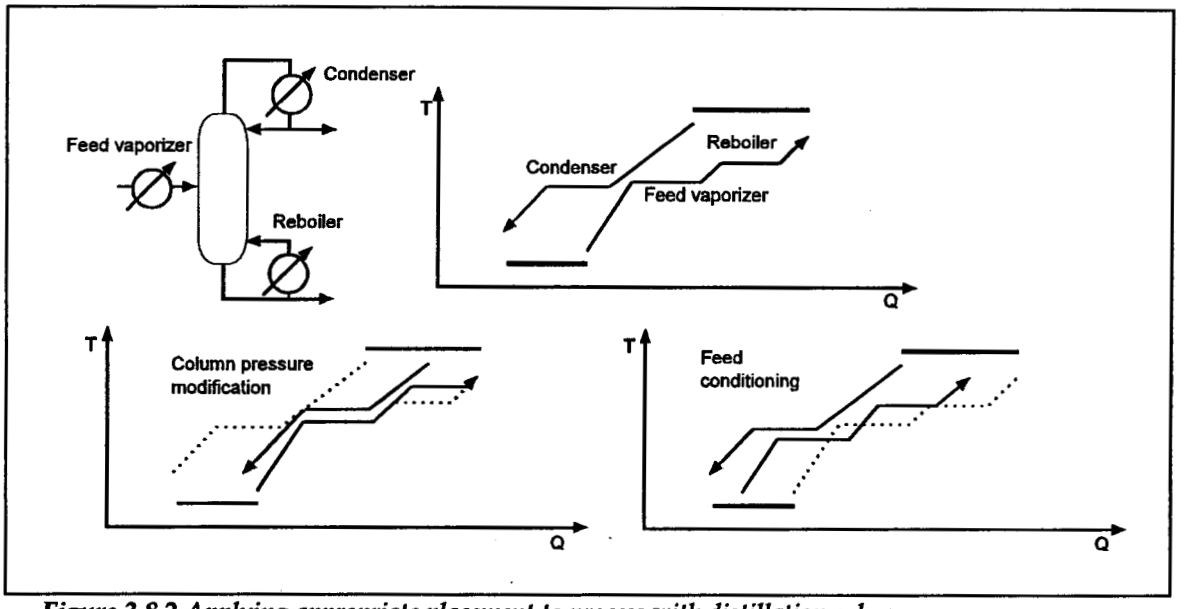


Figure 3.8.2 Applying appropriate placement to process with distillation column.

These guidelines are illustrated with a small example (Smith and Linnhoff, 1988). A process that includes a distillation column with reboiler (REB), condenser (CON) and feed vaporiser (FV) (Figure 3.8.2) is considered. The reboiler and feed vaporiser is placed above the pinch and the condenser below the pinch. If it's possible to raise the column pressure, then the condenser temperature can be raised to above the pinch temperature and the condenser heat can thus be utilised. In this case a hot stream has been moved from below the pinch to above the pinch. Another alternative is to shift the feed vaporiser stream from above the pinch to below the pinch.

3.8.1 Integration of evaporators.

Multieffect evaporators are normally used to effectively evaporate water from a slurry. Using several stages it is possible to decrease the stand alone utility consumption. The evaporator can be described in a T-Q diagram (Figure 3.8.3). This curve will be named Evaporator Grand Composite Curve (EGCC). In Figure 3.8.3 a one-stage and a three-stage evaporator are shown. With three stages the heating demand will roughly be one third of the one stage evaporator heating demand. The heat from each stage can be reused at a lower pressure and temperature at the next stage. The temperature difference from inlet to outlet for each stage is dependent on the heat transfer area in the stage. A small temperature difference requires a large heat transfer area, while a large temperature difference requires less heat transfer area.

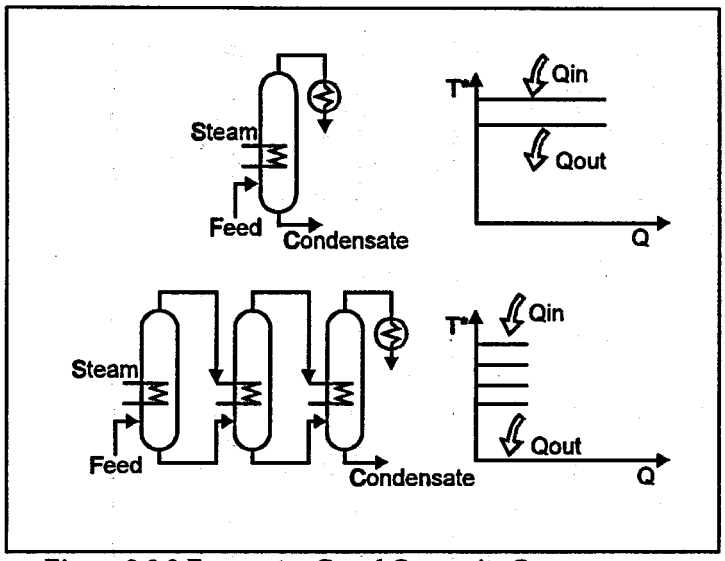


Figure 3.8.3 Evaporator Grand Composite Curve.

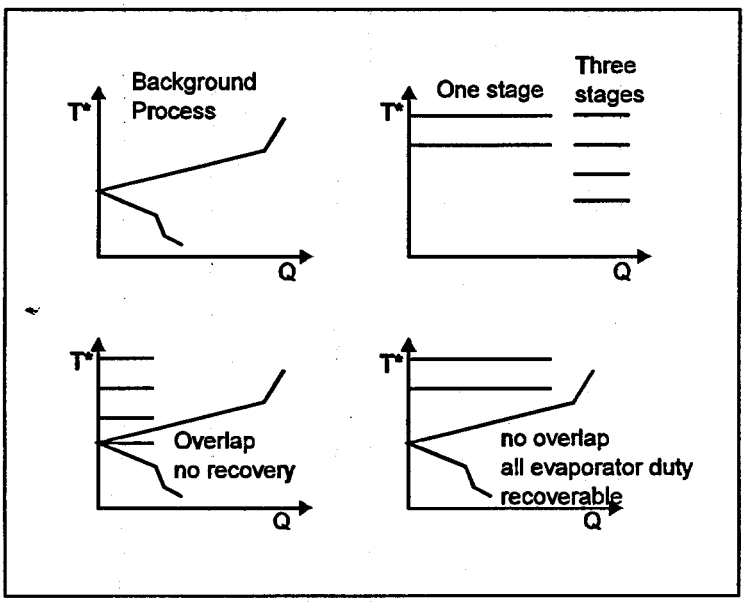


Figure 3.8.4 Modifying evaporator GCC to fit process GCC.

Smith and Linnhoff (1988) used the evaporator T-Q diagram together with the process Grand Composite Curve (GCC) to make an appropriate integration of the evaporator. In Figure 3.8.4 an evaporator is integrated with a process. Two different options are available - a one stage evaporator and a three-stage evaporator. From a stand alone point of view the three stage evaporator only needs 1/3 of the heat for the one stage evaporator. When combining the process GCC with evaporator GCC another result will occur. The three stages evaporator will give an outlet temperature that is too low to serve as hot utility. For the one-stage evaporator the outlet temperature is high enough to serve as a hot utility. In other word: integrating the one-stage evaporator with the process gives no increase in total (evaporator+process) utility demand, while the three-stage evaporator will raise the total utility (both hot and cold) with the net evaporator heat load.

There are generally three degrees of freedom when designing the evaporator (Smith and Linnhoff, 1988)

1. Number of stages.
2. ΔT for each stage.
3. Pressure of each stage.

Varying these parameters, the Evaporator GCC can be modified in order to fit the process GCC for maximum energy efficiency as outlined in Figure 3.8.4. In Figure 3.8.5 the effect of changing number of stages and ΔT at stages is showed on the Evaporator GCC.

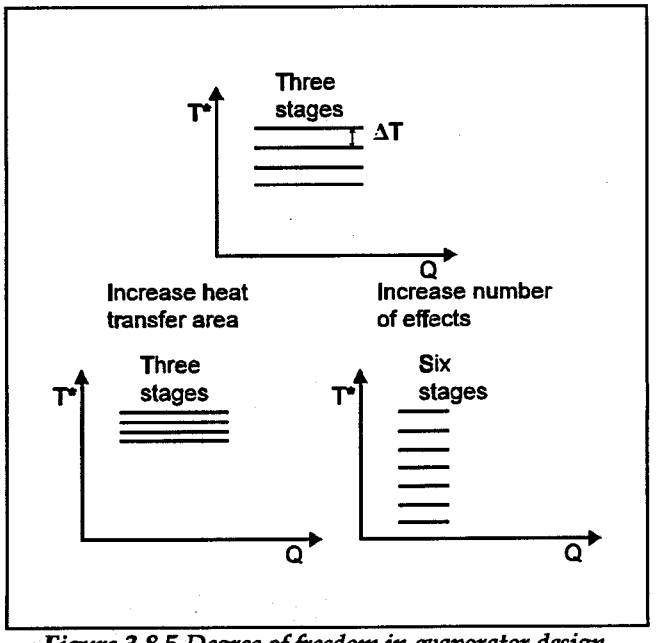


Figure 3.8.5 Degree of freedom in evaporator design.

A detailed description of evaporator design and integration is given by Smith and Jones (1990).

3.8.2 Integration of distillation columns.

In Figure 3.8.2 it was demonstrated how the plus/minus principle was applicable to distillation column integration. There are also developed methods directly for distillation column integration (Linnhoff et al. 1983, Smith and Linnhoff, 1988) and also for distillation column stand alone optimisation (Dhole 1991, Dhole and Linnhoff 1993).

Linnhoff et al. 1983 used the general pinch principle to consider column integration. In that sense the distillation column can be viewed as a kind of heat engine - producing separation work instead of mechanical work. The heat is supplied in the reboiler and discharged in the condenser. Using the principles from heat engine (chapter 3.6) following guidelines can be derived.

Place column fully above or fully below the pinch

Don't place the column across the pinch

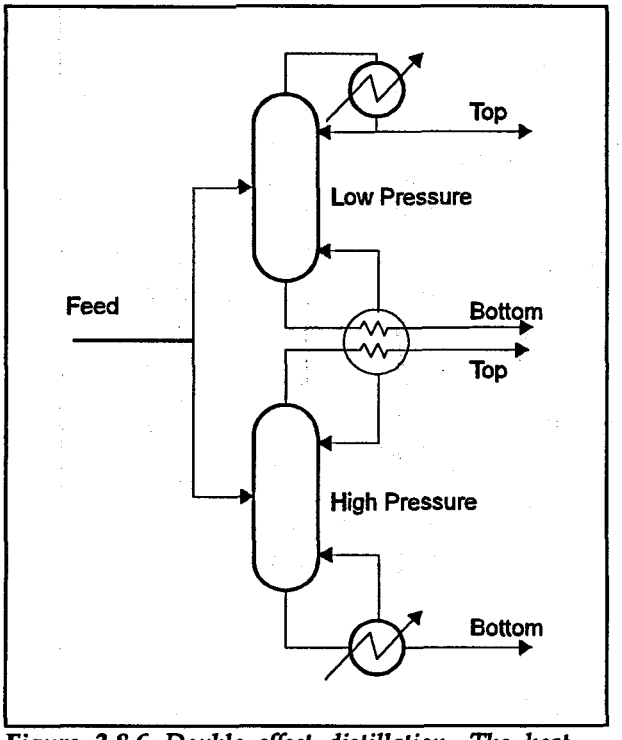


Figure 3.8.6 Double effect distillation. The heat load from condenser 1 is used in reboiler 2.

A method for reducing utility consumption for a single distillation is to use multiple effect distillation (e.g. King, 1971). The multiple effect distillation is similar to the multiple effect evaporation. The feed is split in two or more streams that are fed in separate columns operating at different pressures. If the pressures are chosen correctly, the heat load from the high pressure condenser can be used in the low pressure column reboiler (Figure 3.8.6). The effect of using multiple effect distillation is also similar to the evaporation system. The temperature difference between the reboiler of the first column and the condenser of the last column will be increased when using more columns. When integrating distillation columns into the overall process, this could have a negative effect on the total utility consumption.

Andrecovich and Westerberg (1985) proposed a stacking procedure to minimise utility consumption for column sequences. They represented each column as a box in a T-Q diagram (Figure 3.8.7). Each box can be modified by changing the pressure, number of stages or reflux ratio.

Smith and Linnhoff (1988) adopted the box representation and combined it with the process GCC to get the best heat integration. Using the process GCC it is possible to identify where process heat can be used as column heat duty and where column condenser heat can be used as process heat (Figure 3.8.8). In the figure, four distillation columns are integrated with no additional utility requirement. Again the boxes can be altered to fit the process GCC to minimise utility consumption.

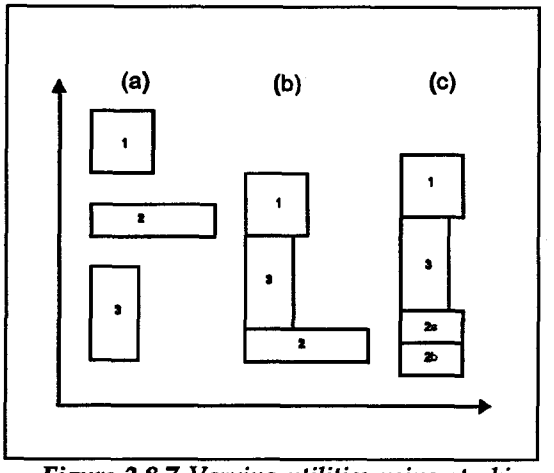


Figure 3.8.7 Varying utilities using stacking procedure: (a) Three columns; (b) stacked configuration; (c) multieffect (after Andrecovich and Westerberg, 1985).

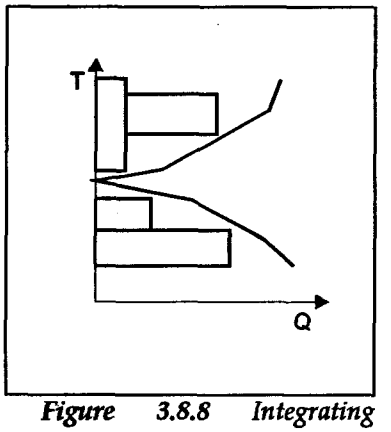


Figure 3.8.8 Integrating distillation columns with background process using box representation.

So far the distillation column has only been represented by the reboiler and condenser load. One change that could increase energy efficiency is the use of side condensers and/or side reboilers. If the box representation is maintained this will result in a notch in the box. This can also be one parameter to use for fitting the boxes to the GCC. Selecting the right side condensers and reboilers can be a tedious affair that demands a lot of column simulations. A more rigorous way is to use the Column Grand Composite Curve (CGCC) as proposed by Dhole (1991). The CGCC can be used to identify the scope for introducing side condensing or reboiling modification, as shown in Figure 3.8.9. The CGCC can be used to set targets for stand alone columns or for process integration.

The approach is to use results from a converged distillation simulation. From the stage values the minimum vapour and liquid flow can be determined. These values can be expressed as enthalpy flow. Then obtain the net heat deficit at each stage temperature and finally cascade the heat deficits to obtain the CGCC.

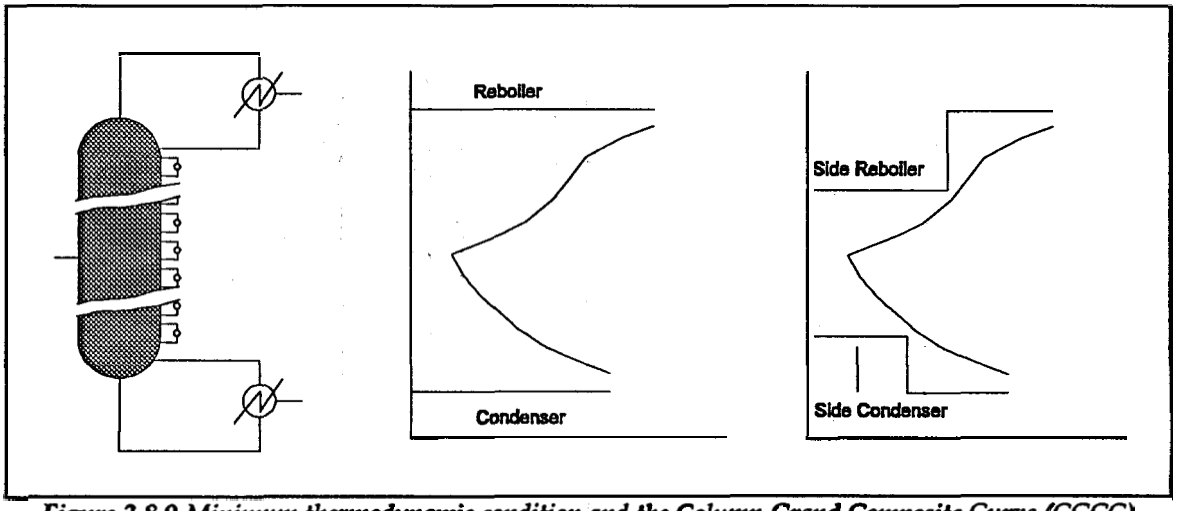


Figure 3.8.9 Minimum thermodynamic condition and the Column Grand Composite Curve (CGCC) (after Dhole 1991).

The basic strategy in the column modification is to reduce the heat and mass transfer loss in the columns (represented by the shaded areas in Figure 3.8.10). Usually, the larger the reduction in this loss area, the greater would be the corresponding energy benefits (Dhole 1991). As for process to process heat transfer there is also a connection between driving forces and equipment size (and thus capital costs).

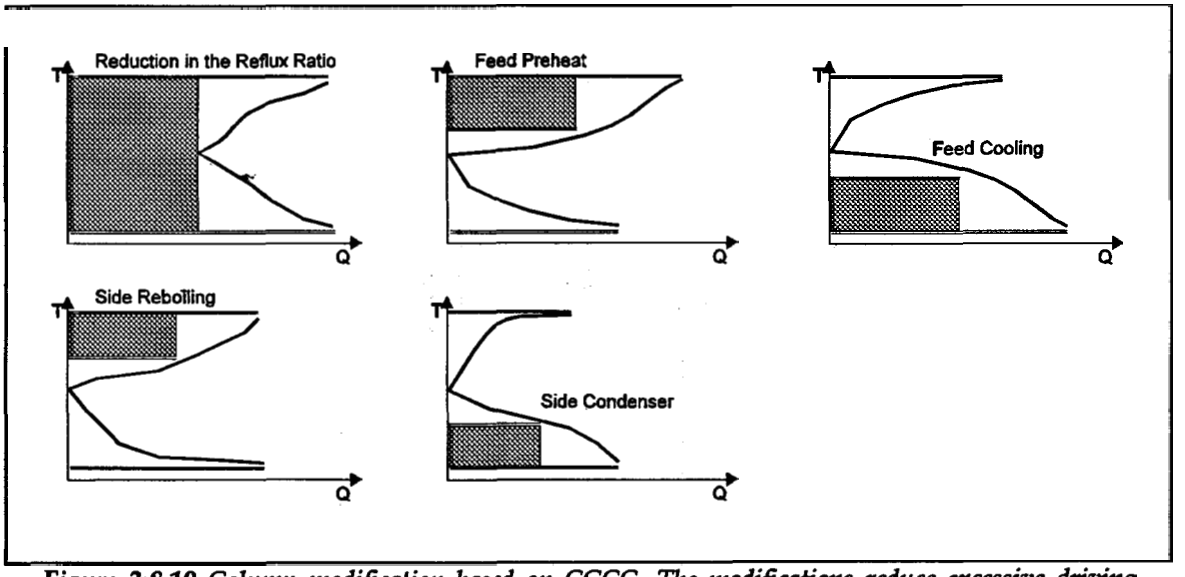


Figure 3.8.10 Column modification based on CGCC. The modifications reduce excessive driving forces (after Dhole 1991).

The difference between using the simple boxes and CGCC when integrating distillation columns with background processes is illustrated in Figure 3.8.11 (Dhole and Linnhoff, 1992). The figure shows an overlap between the process GCC and the CGCC. The box could be lowered by reducing the column pressure and allow the column to be driven by the process heat. But considering the CGCC, reflux reduction and preheating seem more appropriate.

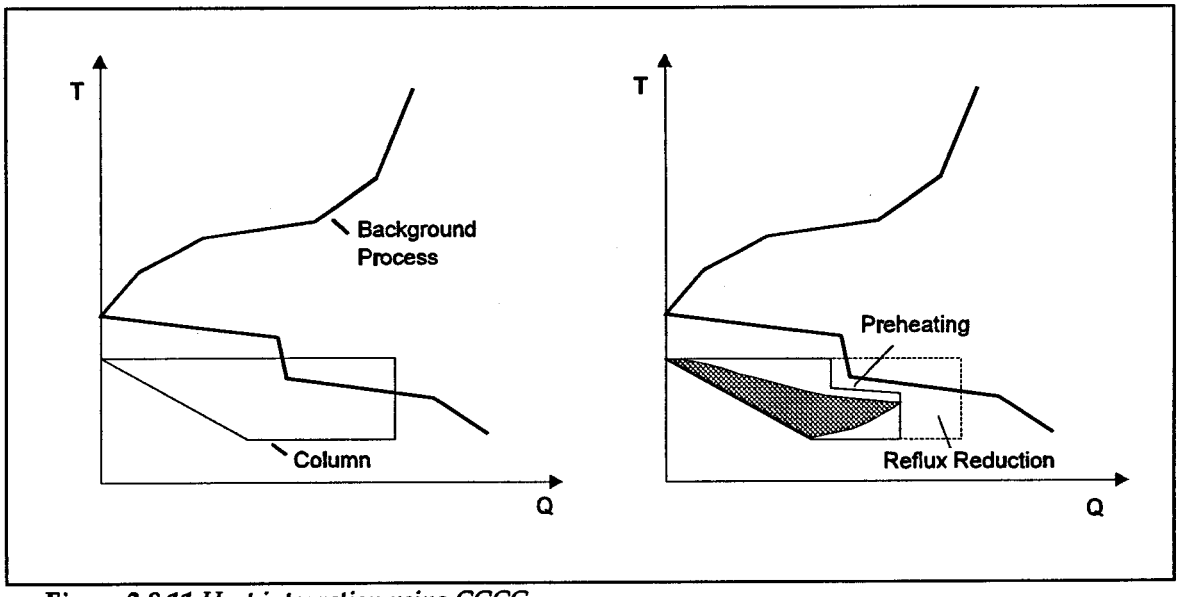


Figure 3.8.11 Heat integration using CGCC.

3.9 Total site targeting.

One of the recent methods emerged from the pinch principles is total site targeting (Dhole and Linnhoff 1993). A typical process site consists of several individual process plants. For several reasons these plants will normally not be heat integrated directly. The plants can have different operation hours, there can be a large distance between the individual plants and the flexibility and operability of each plant will in most cases be affected by heat integration. Finally a more practical problem is that each plant very often have their own organisation (control room, staff etc.).

The way energy can flow from one process to another is via the utility system. The utility system normally delivers and receives steam from individual processes. The total site targeting is an attempt to optimise the total utility system based on information of the individual processes.

The total site can from an energy point of view be considered by looking at the Grand Composite Curves (GCC) for each individual process. The processes are normally served by a central utility system. This is schematically described by figure 3.9.1 (Dhole and Linnhoff, 1993). In most cases the processes are served by several steam mains.

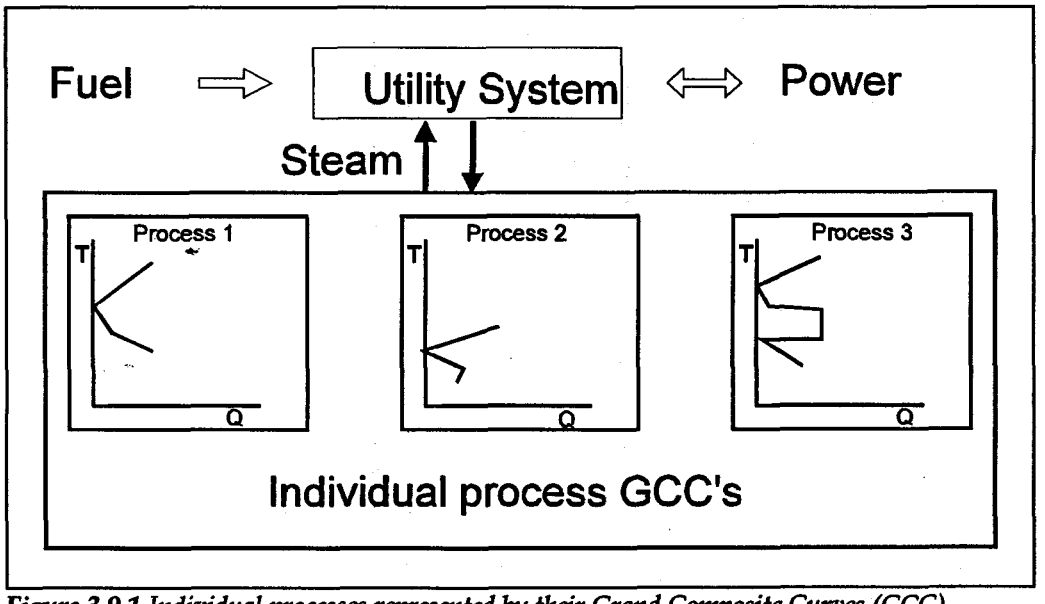


Figure 3.9.1 Individual processes represented by their Grand Composite Curves (GCC).

In the previous chapters the utility levels and co-generation for individual processes have been optimised based on the GCC's. Each of the GCC will suggest different steam levels and loads. Normally only few steam levels within a site will be acceptable. The task on a site wise basis is therefore to locate the most profitable steam levels and co-generation.

The approach will be outlined based on the approach suggested by Dhole and Linnhoff (1993). The basic concept is based on the Site Source Profiles and the Site Sink Profiles. These profiles are constructed from the Grand Composite Curves. The idea is to identify the heat sources and the heat sinks from each process.

The approach is illustrated in Figure 3.9.2 where the GCC's are modified in two steps.

a) The non monotonic parts (pockets) are removed. They represent internal heat exchange.

b) The sources and sinks elements of the resulting GCC are shifted by ½ ΔT_{min}.

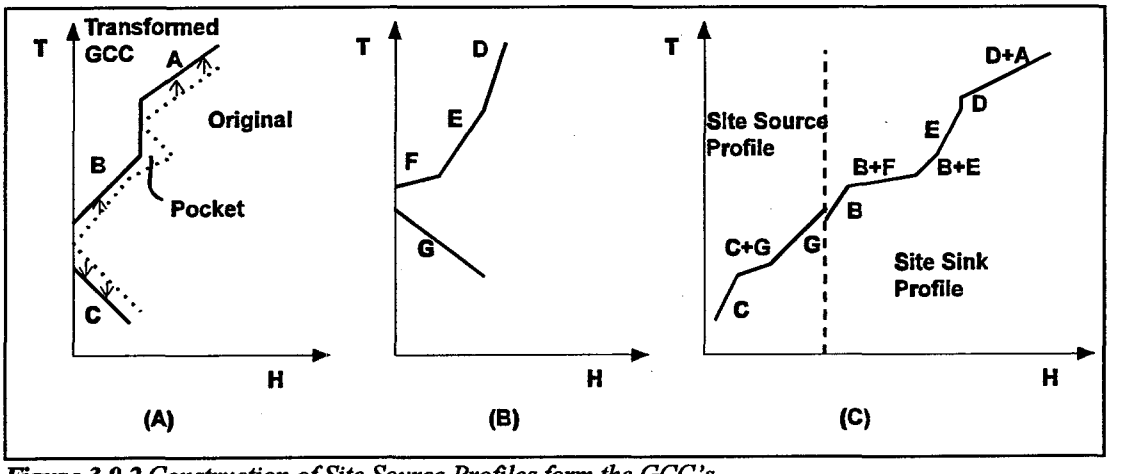


Figure 3.9.2 Construction of Site Source Profiles form the GCC's.

The new modified GCC are now used for construction of the Site Source Sink Profile (SSSP) shown in figure 3.9.2c.

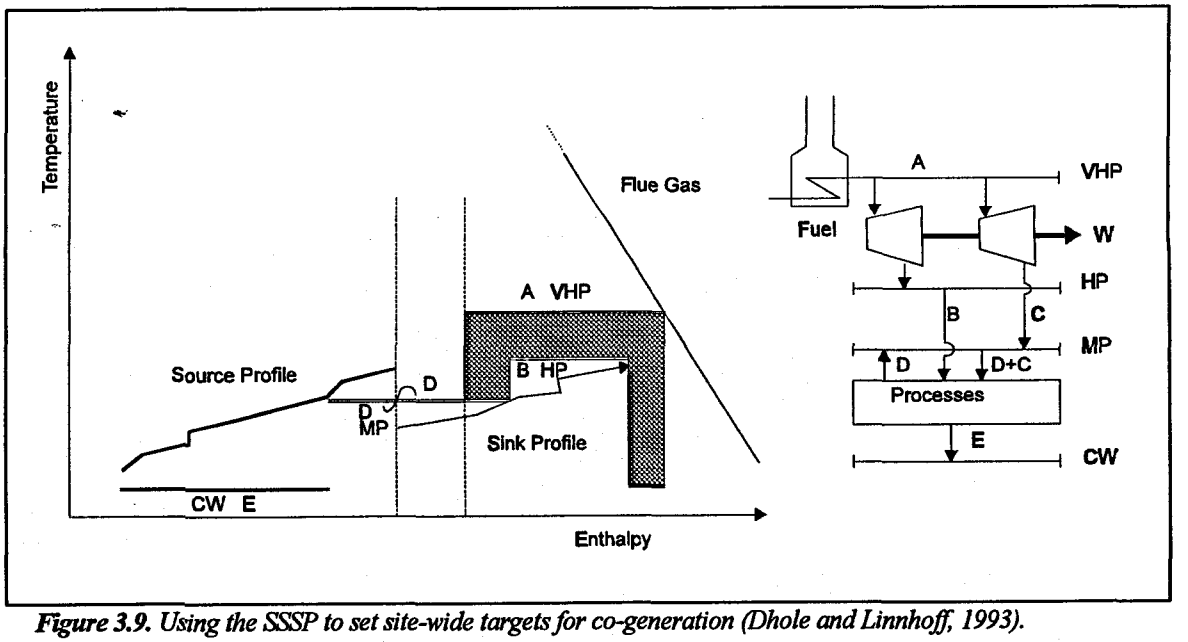


Figure 3.9. Using the SSSP to set site-wide targets for co-generation (Dhole and Linnhoff, 1993).

An example (Dhole and Linnhoff, 1993) is used to illustrate the use of SSSP for targeting total sites. In Figure 3.9.3 a SSSP constructed from a set of GCC is considered. The figure also outlines one possible utility configuration. From the SSSP it is possible to locate the amount of HP, MP-steam and cooling water that is needed/generated at the site. From the SSSP it can be seen that it's possible to generate MP steam from the source profile (D) that can be used in the sink profile. Additional

MP steam must be generated from the utility as well for the HP steam. When the amount of HP and MP steam is determined it is possible to calculate the power generation from the steam turbine. The specific amount of generated power is obtained using turbine simulation.

The total site approach can also be used to evaluate the effect of process changes in individual units. When a Grand Composite Curve is changed the SSSP will change accordingly. The new curve will then disclose the effect from a site point of view.

3.10 Heat exchanger network design.

3.10.1 Grid diagram

An important element in the "Pinch toolbox" is the *Grid diagram* (Linnhoff and Flower 1978, Linnhoff et al. 1982). In the grid diagram - Figure 3.10.1 - each process stream is represented by a straight line. A heat exchanger between two streams is represented by two circles joined by a vertical line. The major advantage compared with the traditional flowsheet representation is that the process stream layout does not change when new matches are inserted. Another advantage is that the downstream order of heat exchangers on a stream is easily identified. As will be showed later the grid diagram also plays a very important role in the network evaluation (e.g. identification of loops, paths etc.). The grid diagram finally also indicates the countercurrent nature of heat exchange.

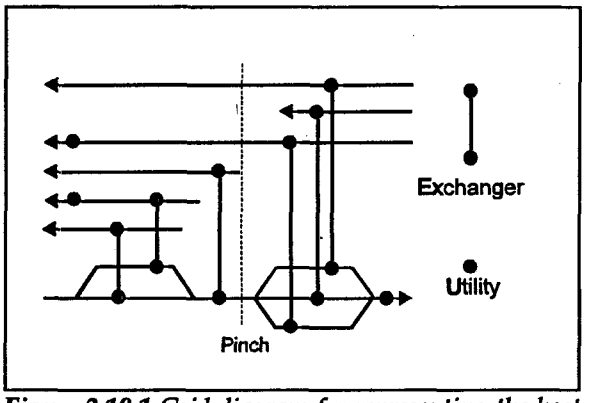


***Figure 3.10.1** Grid diagram for representing the heat exchanger network (Linnhoff et al. 1982).*

It should be noted that the representation in this thesis differs from the original representation. In this thesis the cold process streams go from left to right while the hot process stream goes from right to left, while the original representation is reverse. The alternative representation, which is also used by others (e.g. Dolan et al. 1989, Androulakis and Venkatasubramanian 1991), is chosen to make the temperature axis running from left to right which seems to be more easily comprehended.

3.10.2 Designing Maximum Energy Recovery (MER) networks.

For designing a heat exchanger network that fulfils the energy target found by the problem table (chapter 3.2) Linnhoff and co-workers has derived a set of rules based on the pinch principle (chapter 3.4). First of all the problem should be decomposed at the pinch, since no heat should be transferred from above the pinch to below the pinch. Since it is at the pinch the problem is most constrained (smallest driving force) it is also from here the design should start. To maintain ΔT_{min} the heat capacity flow, that flows away from the pinch has to be lower than the heat capacity flow, that flows into the pinch.

CP_{in} <= CP_{out}

or

CP_{cold} <= CP_{hot} Below the pinch

CP_{cold} >= CP_{hot} Above the pinch

Designing at each side of the pinch individually guaranties maximum energy recovery (MER) subject to ΔT_{min} since cross pinch heat transfer is avoided. Now it is not certain that the CP rules can be met directly if for example no cold stream below the pinch has higher CP than a given hot stream. In that case it can be necessary to split the hot stream into two partial streams.

Another principle that can be derived from the general pinch principles is that the number of streams going into the pinch must be less or equal to the number going out. The reason for this is simply that all streams that are going into the pinch must be brought to the pinch temperature only by heat exchange with another stream on the same side of the pinch. Again stream split can be necessary to fulfil this rule.

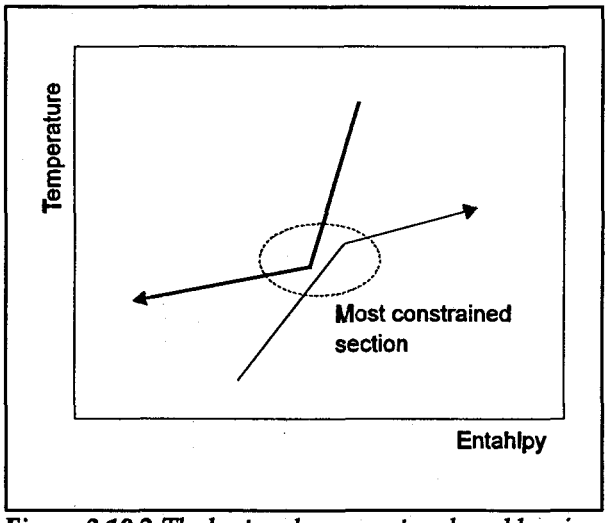


Figure 3.10.2 The heat exchanger network problem is most constrained near the pinch.

As noted the pinch is the most constrained region of the problem. Away from the pinch, the temperature difference between hot and cold streams generally increases. It is therefore simpler here to finnish the heat exchanger network. If the pinch is very distinct (Figure 3.10.2) the MER design will normally also give a near-minimum area. The final network can then be assembled by adding the two partial networks. Although the energy target is met and the area target is nearly met there might be more units in the network than predicted in the targeting part ($U_{min,MER}$).

3.10.3 Loops and paths in heat exchanger networks.

To trade of energy for units Linnhoff et al. (1982) uses Loops and Paths. The procedure for reducing the number of units at minimum energy sacrifice is

1. Identify a loop,

2. Break it by subtracting and adding loads,
3. Recalculate the temperatures and identify the ΔT_{min} violations,
4. Restore ΔT_{min},
5. Repeat for other loop.

In Figure 3.10.3 the steps 1 to 4 are outlined. A loop is identified (a) which is marked with a dotted line. In (b) the heat loads of both exchangers in the loop are gathered in one exchanger. The result of this move might cause a violation of ΔT_{min} (c). By decreasing the heat load (d) ΔT_{min} can be restored. There will, however, be an accordingly rise in heating as well as cooling demand. In Figure 3.10.3 the loop is broken by moving the heat load from exchanger 4 to exchanger 2. It could just as well have been the other way round. Linnhoff et al. (1982) states that it is not possible a priori to determine which will be the best change, but suggest as a rule of thumb to start with the unit with less heat load.

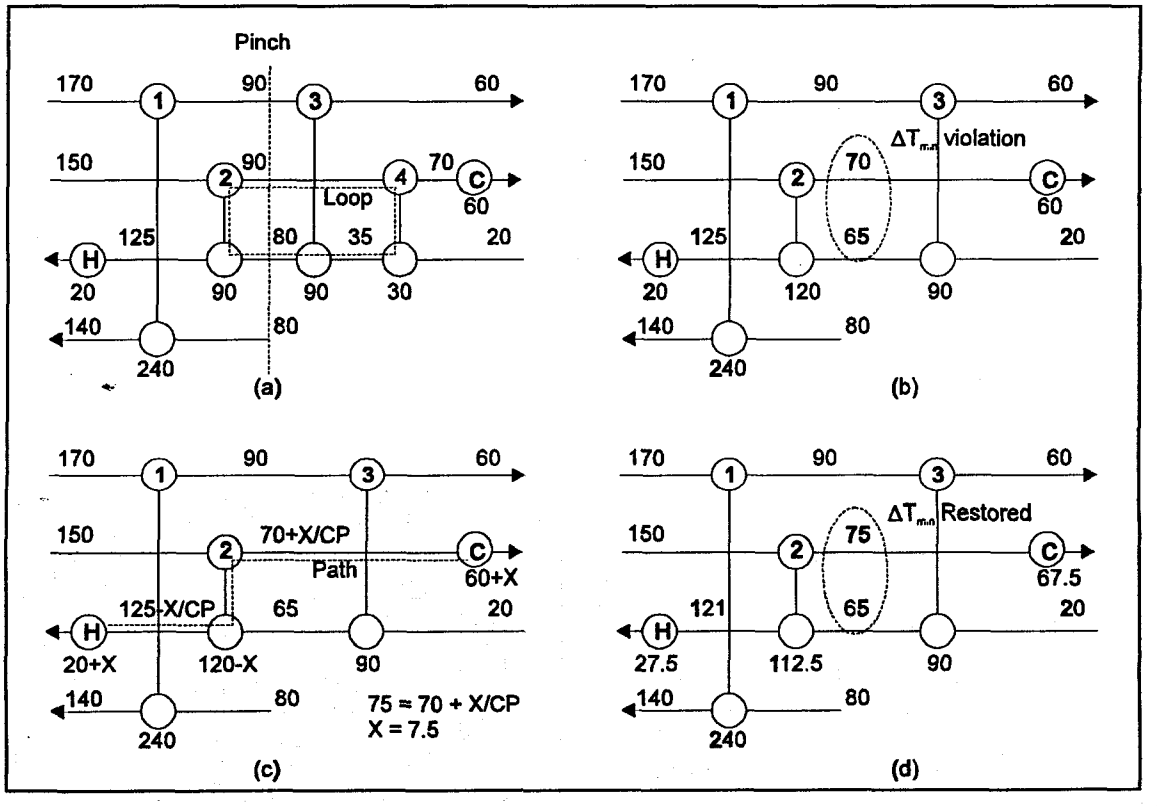


Figure 3.10.3Paths and loops can be obtained by following the streams downstream and through exchangers (Linnhoff et al. 1982).

Loops and paths can be more complex than the example shown in Figure 3.10.3 involving many matches, but the general approach of relaxing energy for units is still the same.

3.10.4 Design for minimum heat exchanger area.

In the above section the procedure for designing a MER heat exchanger network was described, and it was stated that for problems with a distinct pinch the MER initiated with a correct ΔT_{min} would yield a near minimum area network as well. For cases where the pinch is not very distinct, small temperature differences away from pinch also, two tools has emerged that gives guidelines for building near minimum area networks. The first tool is the Driving Force Plot (Linnhoff and Vredeveld 1984, Ahmad 1985) helping the network designer to see whether a proposed match is suitable or not. The second is the Remaining Problem Analysis (RPA) (Ahmad 1985, Tjoe 1985) which gives the designer the revised target after a match is inserted. The basic idea of both tools will shortly be highlighted.

In the area targeting part (chapter 3.3) it was outlined that for problems where all cold and hot streams respectively have the same heat transfer coefficients, the minimum heat transfer area is achieved when the heat is transferred vertically. The Driving Force Plot and the Remaining Problem Analysis are used for analysing the verticality of a proposed match.

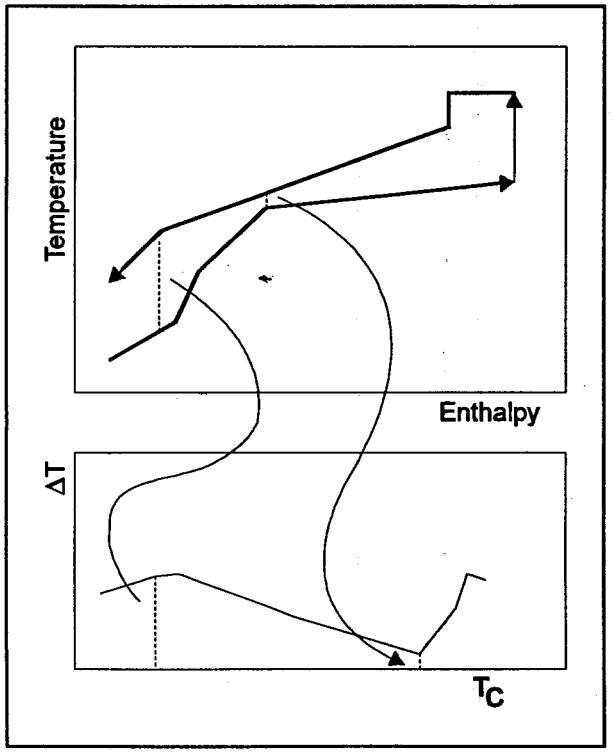


Figure 3.10.4 Driving Force Plot (DFP) can be derived directly from the Composite Curves.

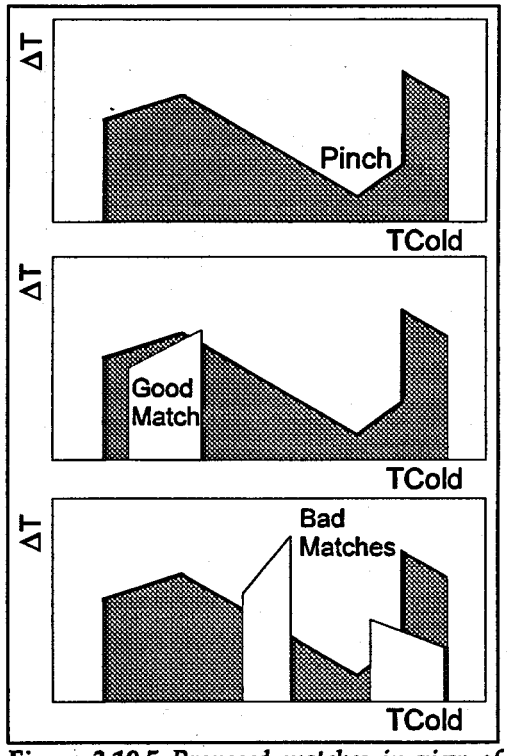


Figure 3.10.5 Proposed matches in view of the DFP plot.

The DFP is derived from the composite curves. Its derivation is illustrated in Figure 3.10.4. The temperature difference at the composite curve is plotted against either the hot or cold composite curve temperature. By plotting the profile of the proposed match on the DFP the deviation from ideal temperature profile can be easily identified. In Figure 3.10.5 three different matches are proposed one of them exhibits good performance while the others more or less misfit. The misfit will actually introduce

some temperature criss crossing (non-verticality) within the design. At the pinch the correct temperature difference will always be the result if the pinch design method for MER design is followed. As mentioned earlier there can be a beneficial trade off between units and energy cost. This will in most cases cause some temperature criss crossing and result in some misfit on the DFP. The main problem using the DFP is that though it gives a qualitative picture of the ideality of the proposed match it does not give any quantitative values of the affect. This is actually best handled using the RPA.

The Remaining Problem Analysis quantitatively calculates the cost implication of a proposed match during the heat exchanger network design. As the name suggests the RPA looks at the remains of the problem after a heat exchanger is proposed. When a match is proposed the two streams that are involved will be cut leaving the remains of the streams together with rest of the streams. The heat exchanger area for the match can be calculated and an energy and area targeting can be carried out for rest of the problems. By comparing the original energy, area and unit target by the remaining problems energy, area and unit target a penalty for the proposed match can be quantified

Unit penalty= 1 + RP unit target - Original Unit target

Energy penalty = RP energy target - Original energy target

Area penalty = Match Area + RP area target - Original area target

The RPA is a simple but powerful tool for evaluating proposed matches. The RPA is especially useful for constrained problems.

The final trade-off between energy, area and units can be done by exploring the loops and paths in the system shifting heat load between exchangers and utilities.

3.11 Retrofitting Heat exchanger network.

While the academic research primarily has focused on methods for design of grassroot heat exchanger network, the majority of industrial cases studies are retrofit problems, where the existing network must be taken into account. In pinch technology the first attempt to make a systematic approach for retrofitting heat exchanger network was made by Tjoe (Tjoe 1986, Tjoe and Linnhoff 1986). Tjoe's approach was based on targeting for the energy recovery, expressed by ΔT_{min}, that best achieve a retrofit project criteria (Pay back, investment limit etc.). The previous work on retrofitting heat exchanger network was mainly based on a comparison between the existing network and a new optimum network. The task was then to evolve the existing network towards the optimum network. More recently Shokoya (1992) suggested a new improved targeting method based on the so called "Area Matrix".

3.11.1 Retrofit by constant area efficiency

The method of Tjoe starts with construction of the energy-area plot - Figure 3.11.1. The plot is constructed by using the problem table algorithm and area target equation for a range of ΔT_{min} values. The curve represents the minimum heat exchanger area for a given energy consumption. The area below the curve thus represents the infeasible area and the area above the non optimum states. By plotting in the actual position of the existing network it is possible to get a picture of the efficiency of the network and thus the scope for improvement.

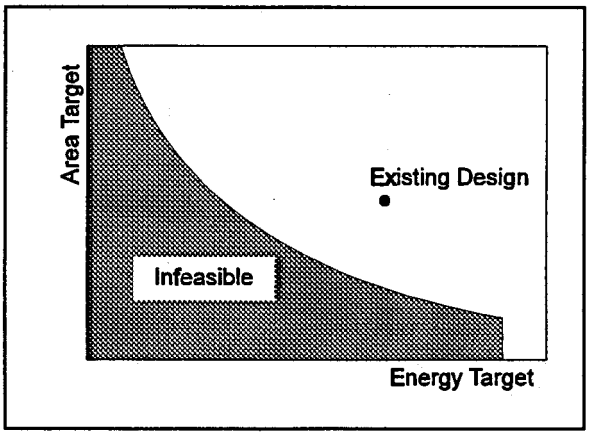


Figure 3.11.1 The energy/area plot relates the minimum area requirement to the minimum energy requirement. The existing network exhibits non-optimality.

In Figure 3.11.2 it is shown that evolving the existing network towards the optimum network for grassroot design will give a reduction in heat transfer area. Since the area is already invested it will probably be more interesting to try to get a reduction in energy consumption by better utilisation of the existing area. The ideal location to aim at would be point A where the minimum energy consumption for the given heat transfer area is reached. However, because of constraints in the existing heat exchanger network, this target is probably too optimistic. Tjoe and Linnhoff (1986)

instead suggested that a more realistic path could be based on an area efficiency (α). This area efficiency could be calculated from the existing network.

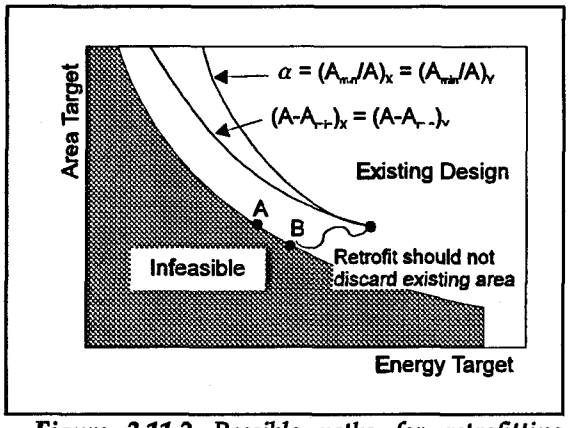


Figure 3.11.2 Possible paths for retrofitting network (Tjoe and Linnhoff 1986, Ahmad et al. 1987).

$$\alpha = \left(\frac{A_{min}}{A_{Existing}}\right) = \left(\frac{A_{tx}}{A_x}\right) \qquad (3.11.1)$$

where A_{min} is the minimum area corresponding to the existing heat exchanger network energy consumption. $A_{t,x}$ is the minimum area corresponding to an improved energy consumption and A_x is the actual expected area for the improved energy consumption. Assuming constant α the additional heat exchanger area for a given energy consumption can be estimated and a trade off between additional area (and thus capital cost) and energy reduction can be established.

Most retrofitting projects are normally constraint by maximum pay back period and maximum allowable investment. Tjoe and Linnhoff (1986) represent the trade off in an investment/savings plot - Figure 3.11.3. Lines of constant pay back are drawn as straight lines. The plot gives a good view of the potential project economics.

It is however noted that the correct retrofit path is very difficult to specify. The constant α is just a very rough estimate of the expected behaviour.

The assumption of constant efficiency for including new area might seem conservative. Ahmad et al. (1987) suggested to use an incremental area efficiency of 1. This will surely give a more optimistic retrofit target than the constant α assumption. The path suggested by Ahmad et al. is outlined in Figure 3.11.2.

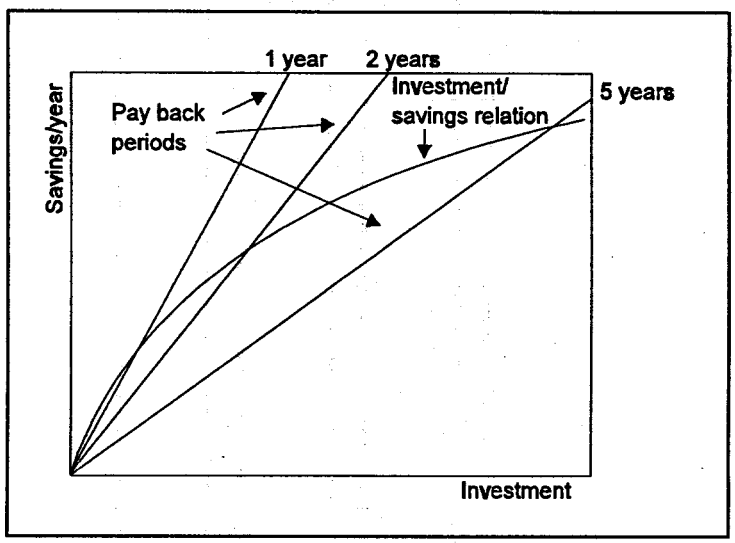


Figure 3.11.3 Investment/Savings plot for retrofit economics.

The pinch design rule for retrofit design of heat exchanger networks has been suggested in the Ph.D. work of Tjoe (1985). The design basically consist of the following steps

(a) *Analysis of existing exchangers.*
Every existing exchanger is analysed for cross pinch heat transfer at a given ΔT_{min}. The contribution from every exchanger to the overall cross-pinch heat flow in the network is determined.

Another tool for analysing existing heat exchangers is the remaining problem analysis (RPA) of area and ΔT_{min}. Where the effect of each existing exchanger is evaluated.

With these to tools the badly placed exchangers are identified.

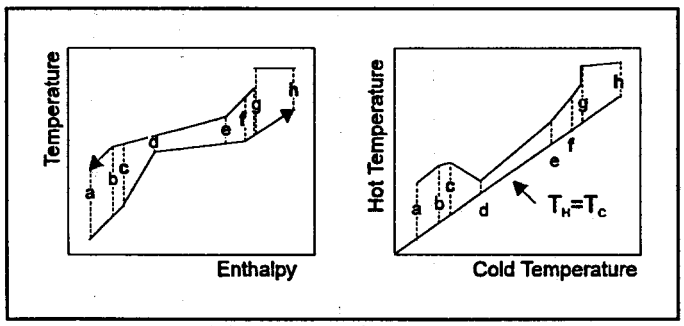


Figure 3.11.4 Modified driving force plot.

(b) *Correction of badly placed exchangers.*
A variation of the driving force plot is used to guide shifting of exchangers. The new plot (Figure 3.11.4) shows the hot composite curve as a function of the cold composite curve.

A bad match, when placed as a straight line in the plot, will not conform with the ideal curve. Shifting the exchanger is done by shifting the temperatures on one side of the exchanger (Figure 3.11.5).

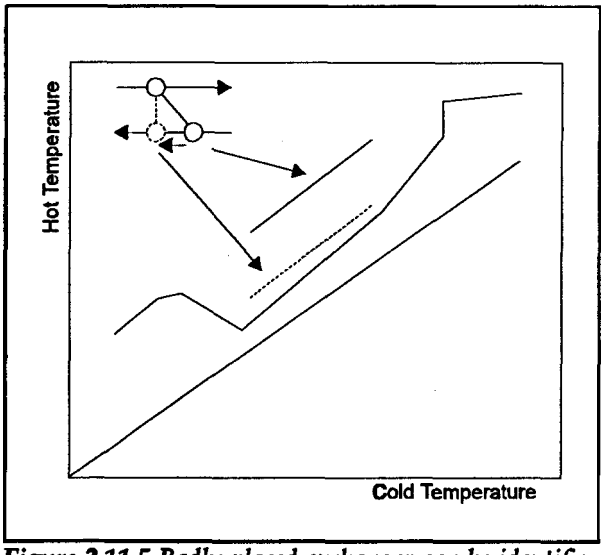


Figure 3.11.5 Badly placed exchanger can be identifie in the driving force plot.

(c) *Placement of new exchangers.*
After the existing exchangers have been replaced, the network is completed by placing new exchangers where the streams' target temperatures have not been satisfied. This is done by the ordinary pinch design rules including driving force plot (DFP) and remaining problem analysis (RPA).

(d) *Evolution.*
The final network is finally evolved using the heat load loops and paths in order to optimise the retrofitted network and to attempt full utilisation of existing equipment.

3.11.2 Area Matrix procedure.

The purpose of the Area Matrix procedure is to give more consideration to the nature of the existing design. This is done by looking in more detail at the total network area calculation. Shokoya (1992) calculates the theoretical heat exchange area between any combination of matches. This is done by looking at the "Spaghetti" network (Figure 3.11.6) and by rewriting the area calculation equation (see chapter 3.3). The spaghetti network is constructed by splitting the streams in each enthalpy interval to allow all hot streams in the interval to exchange heat with all cold streams. The arrangement, that ensures that the available driving forces within the interval is shared equally, is shown in Figure 3.11.6. The distribution of heat loads is a function of the heat capacity flows (CP) ratios of the streams. The area target equation can then be represented as the sum of match area contributions (Eq. 3.11.2).

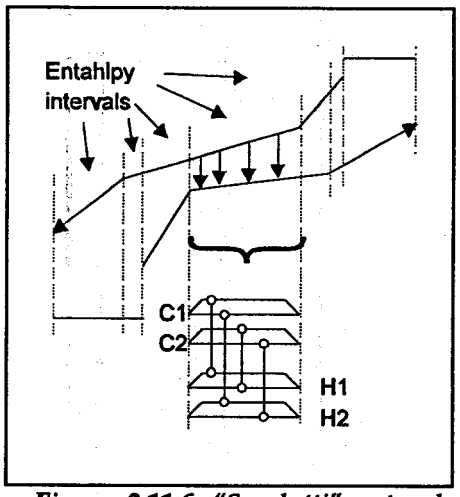


Figure 3.11.6 "Spaghetti" network. Streams are split in each enthalpy interval, to ensure that the driving forces are equally shared amongst the streams (Shokoya 1992).

$$A_{\min} = \sum_{n} \frac{1}{\Delta T_{lm,n}} \sum_{i} \sum_{j} Q_{ij} \left(\frac{1}{h_i} + \frac{1}{h_j} \right) \qquad (3.11.2)$$

The heat load for each match (Q_{ij}) is a function of the total heat transferred in the interval (Q_n).

$$Q_{ij,n} = Q_n \left(\frac{CP_i}{\sum_i CP_i} \frac{CP_j}{\sum_j CP_j} \right) \qquad (3.11.3)$$

The area contribution for the match between cold stream i and hot stream j is then calculated as

$$A_{ij,n} = \frac{1}{\Delta T_{lm,n}} Q_{ij,n} \left(\frac{1}{h_j} + \frac{1}{h_i} \right) \qquad (3.11.4)$$

The total vertical area for matches between cold stream i and hot stream j (A_{ij}) can then be calculated

$$A_{ij} = \sum_{n} \frac{1}{\Delta T_{lm,n}} Q_{ij,n} \left(\frac{1}{h_i} + \frac{1}{h_j} \right) \qquad (3.11.5)$$

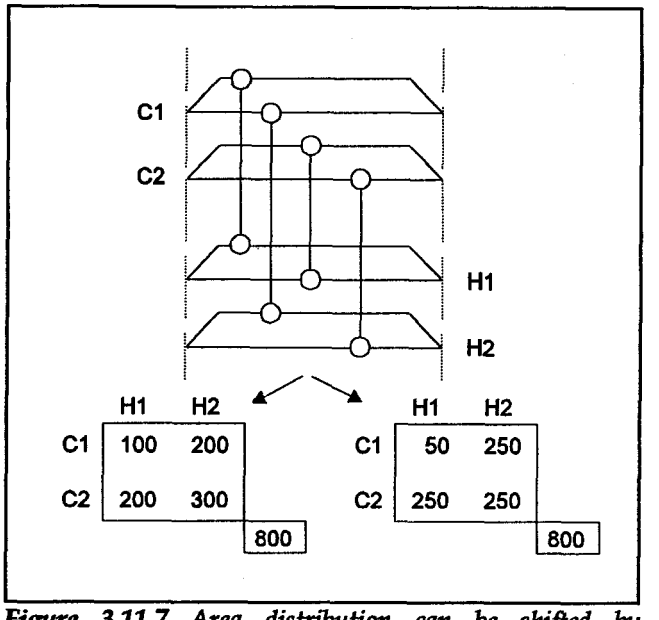


***Figure 3.11.7** Area distribution can be shifted by exploiting the loops within an enthalpy interval whilst maintaining the same total area (Shokoya 1992).*

The Area Matrix is thus created by calculating the contribution from each enthalpy interval for each match combination. For a case with 2 hot and two cold streams this gives a 2 X 2 matrix. The sum of the elements in the area matrix is equal to the total area target A_{min}.

$$A_{\min} = \sum_i \sum_j A_{ij} \qquad (3.11.6)$$

The area matrix represents an ideal distribution of heat exchange area. It is however possible to shift area between elements of the area matrix. This is illustrated in Figure 3.11.7 (Shokoya, 1992), where loops can be used to shift load and thus area between exchangers within an enthalpy interval. There is thus some freedom to exploit.

An area matrix can easily be established for the existing heat exchanger network. The objective is then to maximise the reuse of existing heat exchanger area. Shokoya propose to use a LP formulation to minimise the difference between the target area matrix and the existing area matrix.

3.12 Pressure drop consideration.

Heat exchanger network design procedures make use of information on stream flows, stream heat capacity and initial and target temperature. For capital trade-off a heat transfer coefficient is normally supplied for each stream. The heat exchanger network optimisation is then carried out with the objective to minimise the total energy and capital cost. Pressure drop is then considered afterwards. The trade-off between capital cost, energy and pressure drop has only been considered in depth by Polley and co-workers (Polley et al. 1990, 1991a, 1991b, Shahi 1992). Their works are primarily based on the connection between pressure drop and Reynolds number and the connection between heat transfer coefficient (h) and Reynolds number (Re). For a single phase convective heat transfer under turbulent flow the pressure drop can be expressed in terms of the heat transfer coefficient (Polley et al. 1990)

$$\Delta P = k A \, h^{(3-n)/m} \tag{3.12.1}$$

where A is the heat transfer area, h is the heat transfer coefficient, k a constant that is solely dependent of the fluids physical property. n and m are Reynolds number exponents for heat transfer and pressure drop respectively. With the exponent value m=0.8 and n =0.2 this gives

$$\Delta P = k A \, h^{3.5} \tag{3.12.2}$$

This clearly shows that there exists a trade-off between heat exchanger area and pressure drop. Thus assuming constant heat transfer coefficient one of two non-optimum situations may result.

1. To high pressure drop → high pumping cost.
2. Larger heat exchanger area than necessary.

Beside the pumping/compressing cost there is also an additional size dependent cost for the pump/compressor. Especially compressors are high capital cost equipment. For retrofit design, the trade-off is most likely to be bounded by the existing pump/compressor capacity.

For new plant design Polley et al. (1991) suggests a new area target model based on maximal allowable pressure drop instead of using constant heat transfer coefficients. The new area target model is based on the vertical heat transfer equation (eq. 3.3.3.)

$$A_{\min} = \sum^{stream,j} A_j = \sum^{stream,j} \sum^{interval,i} \left(\frac{q}{\Delta T_{\ln}} \right)_i \left(\frac{1}{h} \right)_j \tag{3.12.3}$$

This equation is based on area contribution, that is the streams' area contribution to the total network area. In the pressure drop model - equation 3.12.2 - it is the total surface area that must be considered. To make use of the pressure drop relationship Polley at al. (1991) uses an estimate of the stream contact area

$$A_{cj} = \sum^{Intervals,i} \left(\frac{q_{ji}}{\Delta T_{lm,i}} \right) \left(\frac{1}{h_j} + R_{opp,j} \right) \qquad (311.4)$$

and

$$R_{opp,j} = \sum^{Streams,k} \left(\frac{CP_k}{\sum^{k} CP_k} \right) \left(\frac{1}{h_k} \right) \qquad (3.12.5)$$

where

A_{cj}	:	contact area of stream j
$R_{opp,j}$	:	the opposing resistance of stream j within a given enthalpy interval
K	:	number of opposing streams to stream j within that interval
CP_k	:	heat capacity flow of stream k
h_k	:	heat transfer coefficient of stream k

Using this expression the total network area is then

$$A_{\min} = \frac{1}{2} \sum^{Streams,j} A_{cj} \qquad (3.12.6)$$

Shahi took the above expression one step further by including heat exchanger fouling. He simply applied the following equation for heat transfer coefficient

$$h_j = \frac{h_{cj}}{1 + R_{fj} h_{cj}} \qquad (3.12.7)$$

where R_{fj} is the specified fouling resistance of stream j.

By solving the area equation 3.12.3 together with the contact area equations 3.12.4 - 5 and the pressure drop - heat transfer coefficient relationship 3.12.2 the total heat exchanger network area can be estimated subject to allowable pressure drop. This actually gives rise to a set of (number of streams + 1) independent equations with the same number of unknown. To solve this problem Shahi suggested an iterative approach.

For the detailed network design Polley and co-workers used the normal pinch design method using the heat transfer coefficients derived from allowable pressure drop. The values are available from the targeting part.

In summary using the pressure drop - heat transfer relationship it is possible to predict the total heat exchanger network cost based on allowable pressure drops. This will

consequently allow for trade off between pumping/compression cost on one side and energy capital cost on the side.

Though the principles developed by Polley and co-workers are sound they do require a large amount of data that are not necessarily available. This together with the absence of available computer tools may prevent the general use of the ideas.

4
HEAT EXCHANGER NETWORK SYNTHESIS BY MATHEMATICAL METHODS.

The aim of HEN synthesis by mathematical methods (MM) is to formulate the optimisation problem mathematically and then subsequently solve it using general optimisation techniques. In the subsequent chapters different approaches will be outlined. The major bottlenecks in the automatic synthesis approach have for long been the discrete decisions and systematic representation of alternatives (Grossmann 1992). Emphasise is therefore placed on these elements.

4.1 HEN representation - Superstructure.

A principal step in synthesis is definition of the search space. This is done in Mathematical Programming by formulating a *Superstructure*. A superstructure is a representation that embeds several alternative configurations. There are several ways of defining a superstructure. A simple example of a manually derived superstructure for the HEN is shown in Figure 4.1.1. The superstructure for this three stream problem is represented by four potential heat exchangers. If the heat load for an exchanger is

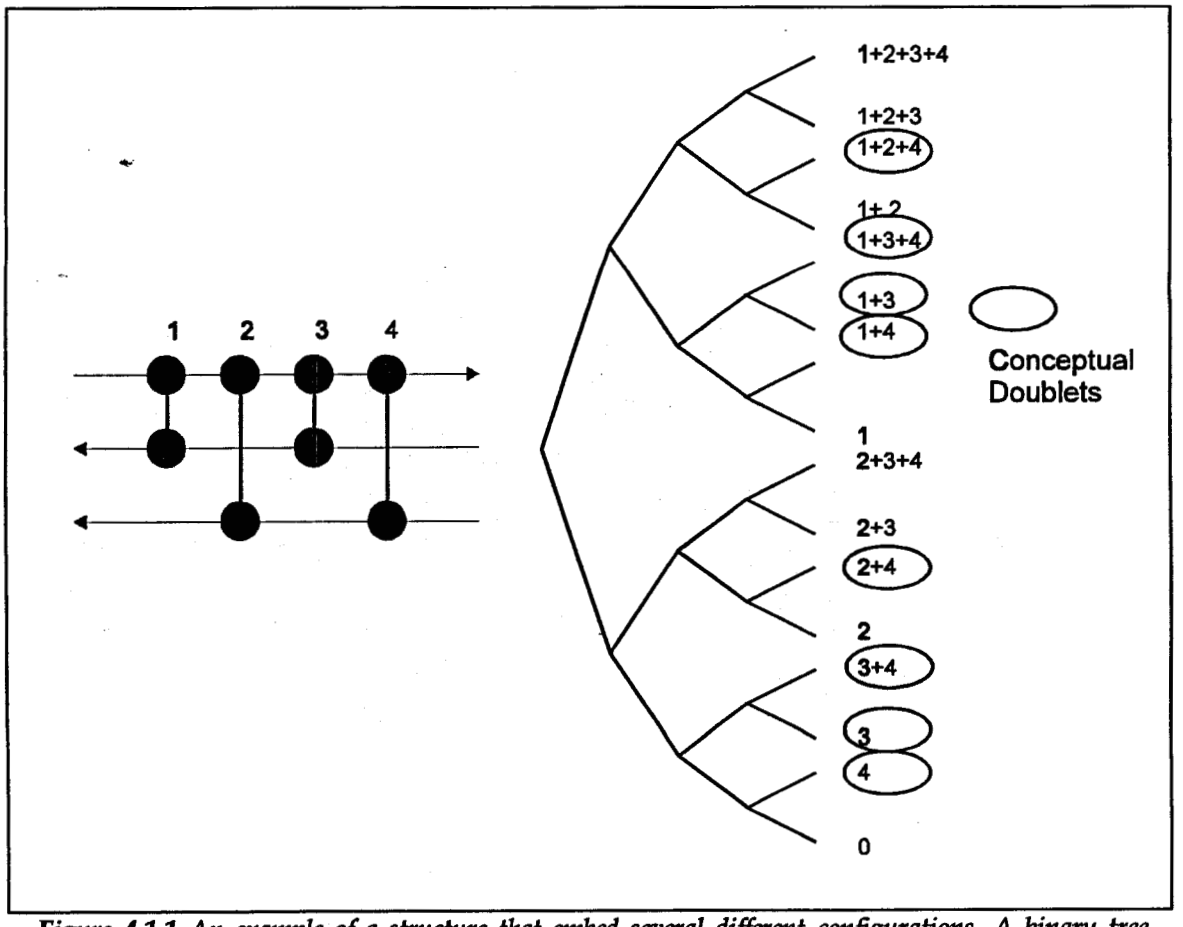


Figure 4.1.1 An example of a structure that embed several different configurations. A binary tree represents the existing of the individual exchangers.

different from 0 then the exchanger exists. The potential configurations for this network representation, can be described using a binary tree where each node represents a subnetwork (Figure 4.1.1). If the tree is traversed 16 potential network is obtained. Excluding the doublet configurations (e.g. 1+2 and 3+4) reduces the number of configurationally different solutions to 8 (including the empty network solution).

Although superstructures can be derived manually for small problems it becomes quite incalculable when the problem size increases. Therefore, it is one of the most significant parts in mathematical programming to handle the superstructure systematically. Floudas et al. (1986) propose a technique that automatically constructed a superstructure for the HEN synthesis problem. The general idea is to predict the minimum number of units (for a given ΔT_{min}) using mixed integer linear programming (Transhipment Model). This model gives the number of units required in each subnetwork (decomposed at the pinch(es)). For each subnetwork a superstructure is derived that allow serial as well as parallel connections (Splits) between the units. An example of a superstructure for a subnetwork is illustrated in Figure 4.1.2 (Floudas et al. 1986). Here one cold stream (C1) shall exchange heat with three hot streams (H1-H3). The Transhipment Model predicts that heat is transferred in three exchangers (C1-H1, C1-H2, C1-H3). It also calculates the amount of heat transferred in each unit. The superstructure is then derived as follows:

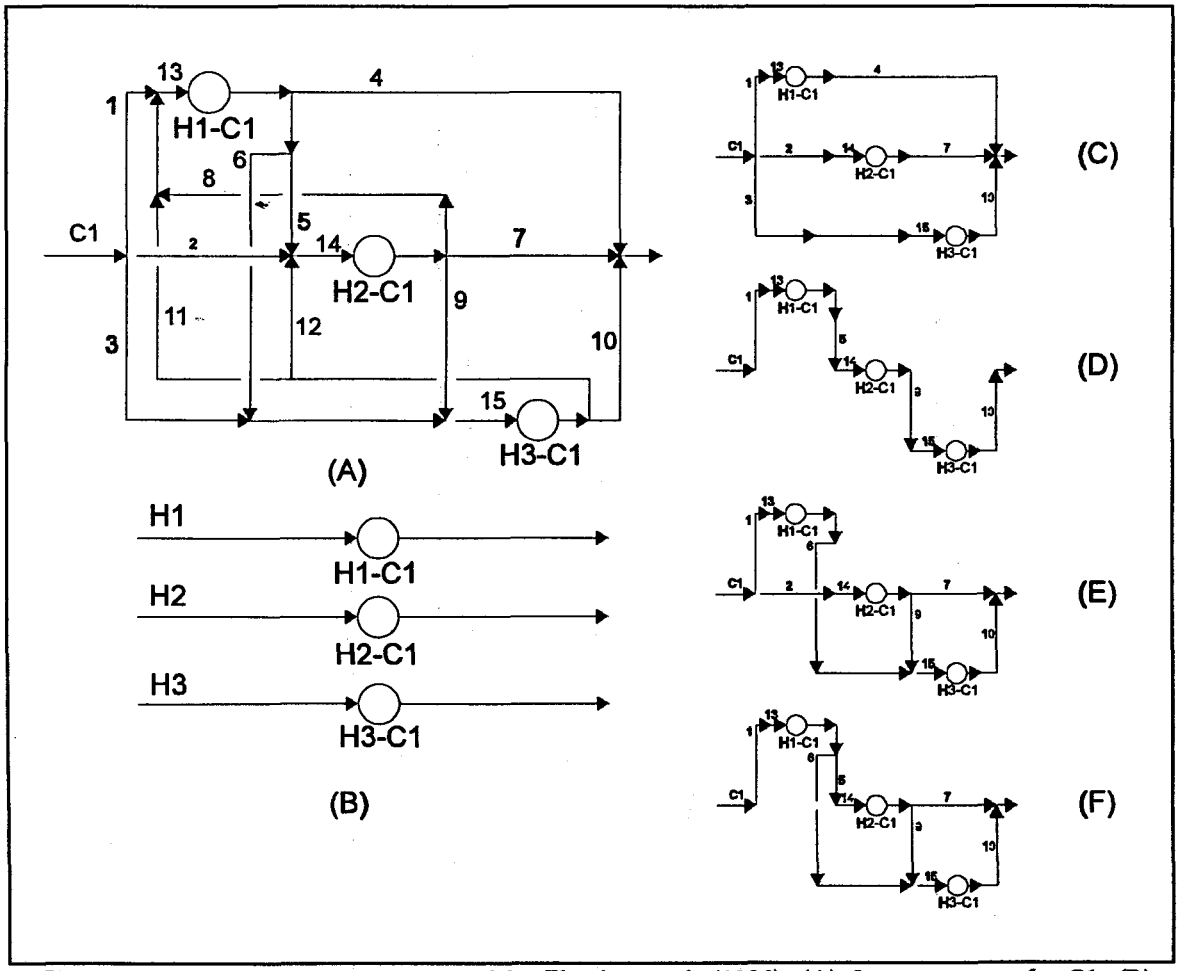


Figure 4.1.2 Superstructure as proposed by Floudas et al. (1986). (A) Superstructure for C1, (B) "superstructure" H1-H3. (c)-(F) Examples of embedded structures..

1. Split the inlet of C1 into three streams that goes to each of the three units.
2. Split the outlet of each unit into three streams such that one goes to the outlet of C1 and the other two goes to the inlet of the other units.

This gives the superstructure for the cold stream (Figure 4.1.2a). For the hot streams, only one match is predicted for each stream. This reduces the superstructure to one exchanger for each hot stream (Figure 4.1.2b). With the constructed superstructure all combinations of HEN structures that obey the Transhipment Model results can be derived. Figure 4.1.2c-f shows some of the possible configurations embedded in the superstructure.

Floudas et al. pointed out that a stream superstructure can be generalised for any number of matches. Each stream superstructure consist of

1. An initial splitting point for the inlet stream that is directed to the inlet of the exchangers.
2. Splitters at the outlet of each exchanger that are directed to the inlets of other exchangers.
3. Mixers at the inlet of each exchanger.
4. A final mixing point for the outlet stream.

The development of superstructures was a major advantage in HEN synthesis. It allowed atomised handling of the configurational aspect. The principle problem with the representation is primarily the difficulties in solving the resulting NLP problem that arises from the formulation. This aspect will be further discussed in the subsequent sections.

An alternative superstructure is proposed by Yee and Grossmann (1990). Their superstructure is based on a sequence of stages in which the hot and cold streams are successively split and remixed. The superstructure is outlined in Figure 4.1.3

The major benefit of this representation is in the underlying constraints that arises. These constraints all become linear thus simplifying solution of the resulting problem.

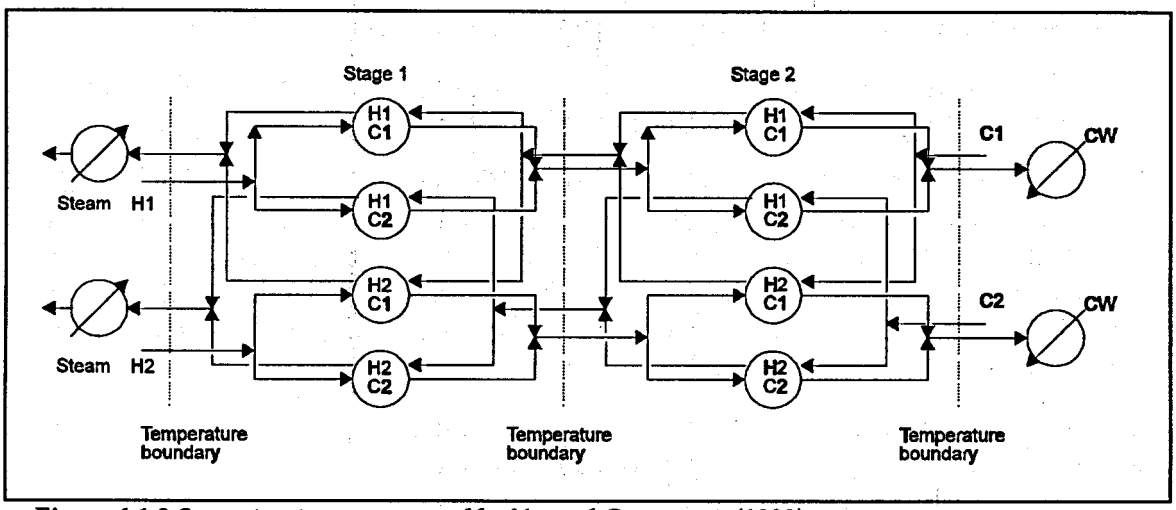


Figure 4.1.3 Superstructure as proposed by Yee and Grossmann (1990).

Finally a different approach to the superstructure is proposed by Dolan et al. (1989). Instead of statically impose a structure that embeds several different configurations Dolan et al. propose a dynamic structure based on a linked list representation. In their representation Dolan et al. treat each side of a heat exchanger as a node in a directed graph. Each node has three pointers that directs to a) the other side of the exchanger b) the upstream node on the stream and c) to the downstream node. Beside heat exchanger nodes Dolan et al. include splitter and mixer nodes. The splitting node has one pointer directed to the downstream node on the split stream and one pointer to the downstream node on the main stream. The last pointer is directed to the upstream node. Finally the combining node has a pointer directed at the upstream node at the split stream, a pointer directed at the upstream node on the main stream and a pointer directed at the downstream node. The superstructure based on the linked list representation is outlined in Figure 4.1.4.

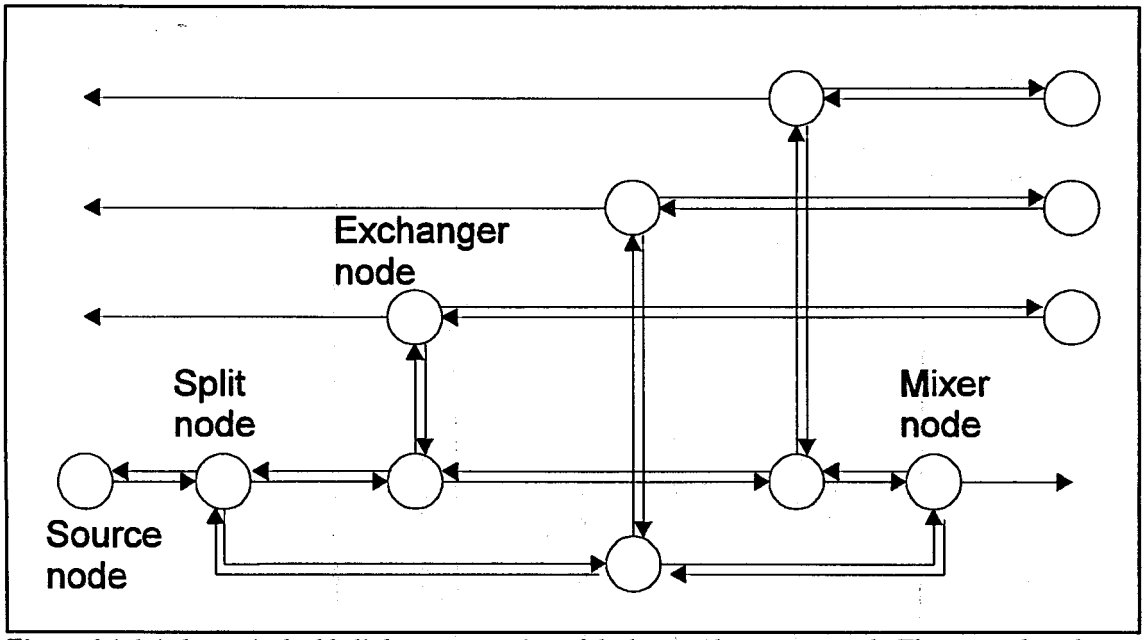


Figure 4.1.4 A dynamic double link representation of the heat exchanger network. The network nodes are interconnected via dynamic pointers (Dolan et al. 1990).

In contrast to the above mentioned superstructures this representation allows for a rigorous representation of all possible configurations without imposing any constraints on number of units and splits. The structure can be changed dynamically during the optimisation search by inserting/deleting nodes and redirect pointers. What is necessary in order to obtain all possible configurations is a well-defined set of search moves. Dolan et al work with six different moves

1. Add new exchanger
2. Delete exchanger
3. Change load of exchanger
4. Switch heat load between two exchangers
5. Add split
6. Change splitratio

Splits are removed automatically when no exchangers are present in them.

The representation proposed by Dolan et al. has been adopted in this work. A further enhancement of the dynamic representation will be discussed in chapter 6.

4.2 Solving the HEN problem using Mathematical Programming.

The equations rising from the HEN model are in their basic form not very complex. To model the HEN, mass and energy balances must be supplied. Under the assumption of constant heat capacity the mass and energy balances can be written as follow

Mass balance splitters and mixers

$$\Sigma F_{in} = \Sigma F_{out} \tag{4.2.1}$$

Energy balance mixers

$$\sum_{in} F_i \; T_i = F_{out} \; T_{out} \tag{4.2.2}$$

Energy balance heat exchangers

$$\begin{aligned} Q &= F_h \, (T_{h,in} - T_{h,out}) \\ Q &= F_c \, (T_{c,out} - T_{c,in}) \end{aligned} \tag{4.2.3}$$

Design equation

$$Q = UA \frac{(T_{h,in} - T_{c,out}) - (T_{h,out} - T_{c,in})}{\ln\left(\frac{T_{h,in} - T_{c,out}}{T_{h,out} - T_{c,in}}\right)} \tag{4.2.4}$$

Further the heat exchanger cost equation

$$CC = C_N + \alpha A^{\beta} \tag{4.2.5}$$

and utility cost equations

$$UC = Q_U \; C_U \tag{4.2.6}$$

Equation (4.2.1)-(4.2.6) constitute the basic equations for the network synthesis. Although the equations appear simple they cause severe problem due to their nonconvex nature. While the equations given here represent the physical behaviour of the HEN a more formal formulation of the problem is given by Floudas et al. 1986.

Solving the network problem requires a method that is able to handle the mixture of continuous and discrete variables. Allthough many attempts were made earlier on, it was first when Linnhoff and co-workers presented their thermodynamic based pinch method that the mathematical approaches really took of. With Pinch Technology, Linnhoff et al. showed that minimum utility, fewest number of units and minimum surface area could be predicted using targeting methods. These principles were adopted in two different approaches. The transportation model by Cerda et al. (1983) and by the transhipment model Papoulias and Grossmann (1983). These methods marked the beginning of the automated sequential approach, where the problem was decomposed into several minor tasks. Papoulias and Grossmann thus based there approach on three steps a) Predict minimum energy cost using a transhipment model (utilising cascade theory from pinch technology) b) use a MINLP model to determine the minimum number of units and the actual matches that should take place in the network c) from the above results construct a network by hand. The approach was later refined by Floudas et al. (1986) who proposed a superstructure and a NLP formulation that solved the last part of the problem that previously had to be solved by hand.

The major benefit in decomposing the problem is the ability to break down the complicated problem into smaller manageable problems. When using a decomposed strategy the assumption is that there is only weak interaction between the different stages in the synthesis. It is now known that this assumption is not fulfilled in general. There does exist a very complex trade-off for energy, capital and number of units that cannot be rigorously decomposed. Different schemes were applied to improve this disproportion. One way is to use an outer loop (e.g. Floudas and Ciric 1989 and Ciric and Floudas 1990). Another way is to use physical insight (Gundersen and Grossmann, 1990)). It is, however, still expected that the better solution is reached if the problem can be addressed expoiting the rigorous trade-off between number of units, utility cost and heat exchanger costs.

While the complexity of the problem is such that the global optimum can never be guarantied it is interesting to see that there in the last few years have been considerable

efforts in solving the complete problem. The major efforts seem to come from the group at Carnegie Mellon University lead by Professor Grossmann. Here Yee and Grossmann (1990) proposed a new approach that based on a simpler superstructure. Quesada and Grossmann (1992) applied a global optimisation technique based on convex non-linear underestimators and a branch and bound search.

Even though major efforts were made, using different schemes of mathematical programming, the first rigorous attempt to solve the non-decomposed problem was made by Dolan et al. (1989,90), who applied stochastic optimisation. They based their work on Simulated Annealing that has proven successful in various fields (Kirkpatrick at al. 1983 and Aarts and Laarhoven 1987). With their intelligent network representation they pointed out a new direction that looks very promising. While Mathematical Programming is very sensitive to the curvature of the problems, Simulated Annealing is almost unaffected by the curvature of the search surface. The search algorithm is based on a modified random search driven only by the objective function.

The Simulated Annealing approach is adopted in the current work and will be discussed further in chapter 5.

With the state of the art methods in HEN synthesis it is most problems in the form described by equations (4.2.1)-(4.2.6) can be solved in a reasonable way (within few percent of the global optimum). These equations, however, do not represent the full practical industrial problems. The design methodologies should therefore not be measured on how efficient they solve the above problem but rather on how they behave on real world problems.

For practitioners the problem specification (4.2.1.)-(4.2.6) does not in general constitute the problems encountered in industry. An obvious limitation of the above representation, that is met commonly, is the assumption of constant physical properties. Further the assumption of counter current heat exchange is too simple for many practical problems. The divergence is especially important when operating with small temperature approaches. Gundersen (1991) pointed out that more rigorous models are needed. In chapter 6 a new fundamental framework for addressing enhanced models based on common industrial problems will be presented.

4.3 Retrofit of Heat Exchanger Networks

Of the intensive research in HEN synthesis in recent years only a limited number of papers have specifically addressed the retrofit problem. This is reflected in the fact that in the thorough review of HEN synthesis by Gundersen and Naess (1990) only one out of about 200 references is directed specifically towards retrofit synthesis. There has, however, in the last few years been a rapid development within this area which still seem to expand.

The retrofit or revamp studies constitutes a far more complex problem than the grassroot design problem. Attention must be paid to the existing network structures and heat exchanger area should be reused as much as possible.

In Pinch Analysis Tjoe and Linnhoff (1986) propose an approach based on a prediction retrofit target based on targeting analysis for the corresponding grassroot problem. More recently a specific approach has emerged (Shokoya, 1992) that takes the existing network layout into consideration. The two methods have been discussed in chapter 3.11.

In mathematical programming it was natural to start out with methods similar to those used for grassroot design. Jones (1986), thus, develops several alternatives for grassroot design. These alternatives are then evolved until they make best use of the existing heat exchangers. Saboo et al. (1986) uses a sequential approach, where the first step is to analyse the existing network using energy and area targeting. Comparing the results it is decided whether or not to proceed to the next stage. In the next step it is analysed whether it is possible to increase performance by increasing the sizes of the existing exchangers. This is done under the assumption that it is cheaper to modify existing exchangers than to insert a new exchanger. Finally structural changes are considered based on engineer driven modifications and automatic evaluation. In that way several alternative solutions are obtained and from comparison with existing area distribution the best solution is picked up. The sequential procedure is build in a user driven computer program RESHEX (Saboo et al. 1986). The program is build upon a range of targeting and synthesis procedures and can handle grassroot design as well as retrofit.

Ciric and Floudas (1989) proposes a two step approach. In the first step a MILP formulation is used to address the assignment problem. Solution of this formulation provides information on which exchangers should be changed and/or reassigned and where new exchangers should be placed. From the result of the first stage a superstructure is derived. The second step is to apply a NLP formulation for the superstructure. The solution of the NLP gives a proposed optimal retrofit design. The minimum approach temperature is applied at the initial stage but relaxed in the NLP model. An outer loop is applied to optimise the initial approach temperature. Ciric and Floudas specifically accounted for six different structural modifications which is categorised as

1 Existing exchanger is placed in original position
2 Existing exchanger is placed in another existing exchangers place
3 Existing exchanger is placed in a new position (1 stream is the same)

4 Existing exchanger is placed in a new position (none of the stream are the same)

5 A new exchanger is placed in a position previous occupied by an existing match

6 A new exchanger is placed in a new position

The different categories require different piping changes. Ciric and Floudas (1989) accounts for the piping cost by applying cost factors for each category of changes. This is added to the cost functions for heat exchange area purchase in the objective functions.

The solution procedure used by Ciric and Floudas follows the grassroot techniques, starting by optimising in stages: First utility consumption then number of units and finally area. This also gives the major disadvantage of the method which is similar to the limitation of the earlier grassroot techniques. The method is not capable to perform simultaneous trade-off between structural modification and utility requirement. Later refinement (Ciric and Floudas 1990) applies a MINLP formulation where the simultaneous trade off between area and number of unit is included. This is combined with an outer loop where the energy (in terms of minimum approach temperature) is traded against capital.

Yee and Grossmann (1991) took the retrofit procedure one step further by enhancing the second step in the procedure by replacing the NLP formulation with a MINLP formulation. They thus handle the simultaneous energy-unit-area trade-off. Further they include a presreening stage, where the economical feasibility of the retrofit project is determined. The major problem with the new formulation is the high complexity of the formulation. Solving a simple example with 2 cold stream and 2 hot stream with 5 existing units requires (depending on solution procedure): 299 constraints, 169 variables and 65 binaries (Yee and Grossmann 1991). Since the general formulation is nonconvex it is not possible to guarantee that a global optimal solution can be found. To overcome the difficulties Yee and Grossmann applies several approximations.

To solve the problem of retrofitting or revamping heat exchanger network it is important to develop a framework that includes all essential factors and constraints. The majority of the presented methodologies are still relying on the simple problem formulation described in chapter 4.2 although with additional modifications for costing. For problems with non-constant heat capacities, no-countercurrent heat exchangers there is no general methods available.

4.4 Flexibility, operability and other aspects of the HEN synthesis problem.

So far the discussion on HEN synthesis has been based on methods aimed at solving the traditional HEN problem constituted by equations 4.2.1 to 4.2.6 with additional terms for the retrofit problem. There has, however, been a development towards implementing additional elements in the synthesis problem. In this section the focus will be put on the following aspects

- Flexibility - The ability to operate under changing conditions.
- Operability - The ability to handle dynamic changes for example during start up.
- Non constant properties - Ability to work with temperature dependent properties.
- Enhanced heat exchanger models - Working with more detailed design equations and cost functions.
- Piping and pressure loss consideration - Including additional aspects to the general HEN synthesis problem.

4.4.1 Flexibility.

Several papers treat the flexibility aspect of the HEN problem. Saboo at al (1986a,b) uses the term *resilient heat exchanger network* to describe a HEN that is able to deal with varying operating conditions and remain controllable. In their approach, implemented in the software package RESHEX (RESilient Heat Exchanger network analysis and synthesis), they treat the flexibility aspect at a post synthesis level. That is for a synthesised network a resilience analysis is carried out based on a specified disturbance range. The network is defined as resilient if it is operable with utility loads deviating by less than a specified amount from the MER (Maximum Energy Recovery). They further introduce a so-called Resilience Index (RI). This value is defined as the maximum arbitrary disturbance load a network can tolerate, while still meeting the target temperatures within a specified heat target and minimum approach temperature. The RI is then used to aid the designer in selecting among alternative designs.

Later Colberg et al. (1989) showed that a general resilient target can be generated before design. They show how an uncertainty range on uncertain parameters influences on the Composite Curves. Considering these observations they make a distinction between *Class 1* and *Class 2* uncertainty ranges. In class 1, the uncertainty ranges do not change the stream population above and below the pinch. This is the case when it is the same stream that causes the pinch for the complete uncertainty range. The class 2 uncertainty range is on the other hand uncertainty ranges where there is a shift in which stream causing the pinch. In their approach Colberg et al. (1989) limit themselves to class 1 uncertainty ranges. They argue that class 2

uncertainty ranges generally require more complex HENs than class 1 uncertainty ranges.

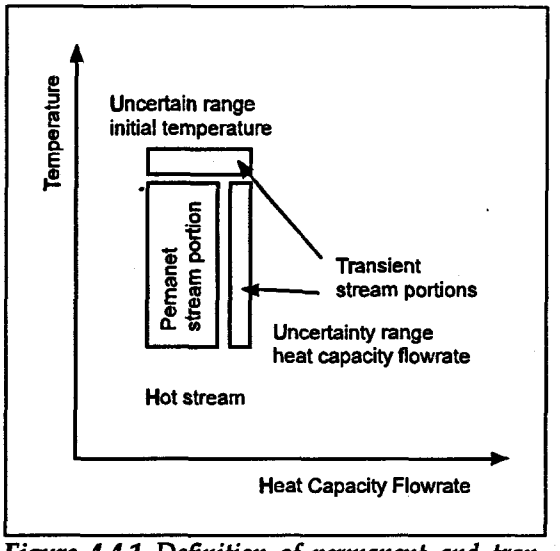


Figure 4.4.1 Definition of permanent and transient stream portion.

The transition point between class 1 and class 2 uncertainty ranges is denoted *critical uncertainty point* (Colberg et al. 1989). It is at this point the problem is assumed to be most constrained. Colberg et al. shows how the resilient targets can be used in the synthesis stage. First they locate the critical uncertainty point. Then they design HEN's for both the nominal cases and for the critical case. These structures are finally merged into one structure. The resulting structure is able to handle the nominal point as well as the critical point. By calculating a resilience index for the desired uncertainty range it is possible to test whether the network is resilient throughout the uncertainty range.

A somewhat similar approach has been proposed by Cerdá and co-workers (Cerdá et al. 1990a, Cerdá and Galli 1990b and Galli and Cerdá 1991). Here they distinguish between convex and non-convex network problems. In a convex HEN problem the pinch stays fixed or moves continuously tied to an uncertainty range (Galli and Cerdá 1991). They propose methods for synthesis of both convex and non-convex HEN synthesis problems. Cerdá et al. (1990a) partition all streams into permanent stream portions and transient stream portions. The permanent stream portion of a stream is the part that is always present. The permanent and transient stream portions are illustrated in Figure 4.4.1 (after Galli and Cerdá 1991). For a hot stream the permanent part is from the lowest allowable inlet temperature to the target temperature and likewise the minimum allowable heat flowrate. The rest belong to the transient portion which represent situation that can be encountered during operation. Galli and Cerdá (1991) gives an eleven step procedure for the general synthesis of flexible HENs. In short they start by defining the disturbance ranges for the process streams and split streams into permanent and transient portions. They then discover a set of dominant pinch points controlling the network design. This is done by looking at the

heat cascade (see chapter 3.2) for the permanent stream portions as well as for the transient portions individually. The problem can be solved with a LP transhipment model (Galli and Cerdá 1991). The next step is to determine the number of necessary units and placement of these (on subnetwork basis). This ends up with a MILP problem which is formulated based on the pinch domain set. From this point the problem is solved using standard procedures for HEN synthesis based on fixed streams.

What has been seen so far is an attempt to include the flexibility aspect into the HEN synthesis. Both Colberg et al. (1989) and Galli and Cerdá (1991) base their approach on the assumption that the optimal HEN features maximum energy recovery (MER) with regard to a specified minimum approach temperature (ΔT_{min}). Further none of the approaches seem to handle the flexibility at a rigorous level, where the flexibility is included in the objective function. In general the flexibility can either be handled as constraints or be included in the objective function (or both). There is though an obvious challenge in incorporate flexibility at a more detailed level e.g. by applying probabilities to the operation conditions. This could be done using distribution models or by lumped values.

4.4.2 Operability and controllability in HEN synthesis.

In chapter 4.4.1 the static flexibility aspect of the HEN synthesis problem is discussed. Calandranis and Stephanopoulos (1988) include the dynamic aspect of HEN. They claim that operability and controllability are issues of utmost importance because the network represents energy transfer between different process units. Calandranis and Stephanopoulos (1988) suggest an approach for designing control loops and further an approach for sequencing the control action of the loops. Considering structural considerations they come up with a set of guidelines. The available manipulated variables treated are: Exchanger by-pass flow rate, utility loads and when present stream split ratios. The guidelines are divided into two, treating static respectively dynamic considerations.

> **Static considerations** *Maintain only feasible alternatives.* A feasibility test validates if disturbances can be handled staticly. *Prefer paths involving a smaller number of heat exchangers.* Using that guidline only a small part of the network is disturbed when a transition in steady state operation takes place.

> **Dynamic considerations** *Prefer routes involving dynamic elements with smaller delays and time constants.* In general it is preferable to keep the network transient for as short a time as possible. *Avoid paths that dynamically interfere with important outlet temperatures.*

These considerations refer to design time issues. Calandris and Stephanopoulos also discuss the importance of dynamic screening of paths at operation time and how to implement the selected control paths. Much of the discussion is based on example

heuristics and they conclude that a knowledge based system is the only appropriate paradigm for computer implementation of their approach.

4.4.3 Property model in HEN synthesis.

In section 4.2 it was mentioned that the problem specification equations. 4.1.1 - 4.1.6 does not constitute a real industrial problem. One of the major simplifications is the assumption of constant heat capacity which in many cases is far too crude. Despite of this only few publications has treated this problem explicitly. Allthough the extension from constant properties to temperature dependent piecewise constant properties seems to be straight forward, it is still to be evaluated what effect such an extension will have on solution procedures i.e. convergens properties.

Dolan et al. (1990) mentioned that their approach using Simulated Annealing could be extended to handle temperature dependent heat capacity and film transfer coefficients. Jezowski (1992) apply three general equations for expressing the enthalpy change (ΔI) as function of temperature in the SYNHEN synthesis package.

$$\Delta I = \int_{t_1}^{t_2} [a + bt + ct^2 + e\frac{1}{t}]dt$$

where a, b, c, e are parameters for a stream.

$$\Delta I = \int_{t_1}^{t_2} \left[\frac{0.403}{\sqrt{\rho}} K1 + \frac{0.009}{\sqrt{\rho}} K1t\right]dt$$

where ρ is the relative density for the oil fraction and K1 is the Watson factor.

Finally Jezowski allow for a piecewise linearised model.

$$\Delta I \text{ from interpolation in arrays } I = f(t)$$

4.4.4 Heat Exchanger Modelling in HEN Synthesis.

In most HEN synthesis studies it is assumed that heat is transferred counter currently. Since industrial use of true counter current heat exchangers are limited it is necessary to correct the results obtained assuming counter current heat exchangers. The magnitude of such acorrection is dependens on what type of heat exchanger is wanted and the log mean temperature difference. In some cases, especially with small approach temperatures, there is risk that the derived solution is impractical or even

infeasible. To illustrate this aspect the solution from Dolan et al. (1990) to the 7SP4 problem is evaluated for a detailed exchanger design (Figure 4.4.2).

It is noted that the minimum temperature difference in the network is 2.5 °C. If a single pass 1-2 exchanger is to be used the solution of Dolan et al. is infeasible. Applying a multipass heat exchanger the solution becomes feasible with a high number of shells. Using the approach suggested by Ahmad et al. (1988) with a specified $X_p = 0.9$ (see section 3.7) an exchanger with 47 small shells is found. Thus it is very unlikely that this solution will be optimal.

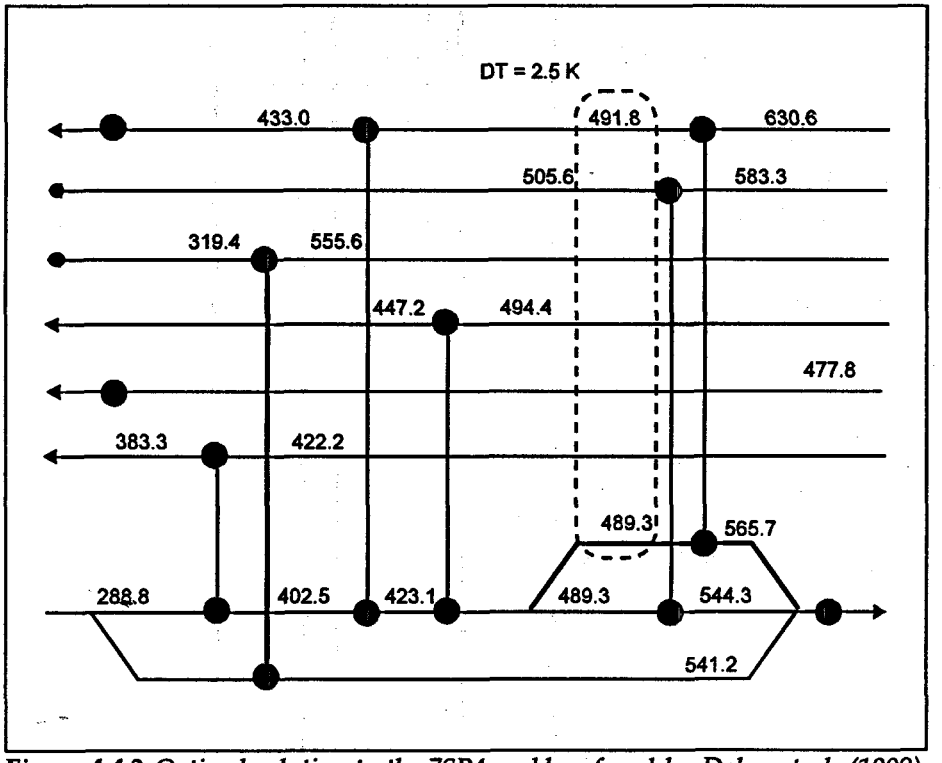


Figure 4.4.2 Optimal solution to the 7SP4 problem found by Dolan et al. (1990). Detailed heat exchanger design will reject the proposed design.

The above example is a case where the heat exchanger modelling is of major importance. It is on this background surpassingly how little attention the modelling aspects have been given.

4.4.5 Additional aspects of the HEN synthesis problem.

Pressure drop consideration has been mentioned shortly in chapter 3.12. In mathematical synthesis the problem of pressure drop seems to be virtually unexploited. Shahi (1992) demonstrated through examples that not taking pressure drop into consideration can lead to serious design mistakes. He showed that there is a clear connection between allowable pressure drop and heat transfer coefficient. This can especially be important when investigating retrofit problems.

Another aspect almost untouched is the physical layout of the heat exchanger network. Zhelev (1994) pointed out that taking the physical placement of heat

exchangers into account and thus find correct piping costs could change the optimum solution.

5
SIMULATED ANNEALING FOR HEN SYNTHESIS

In this chapter the application of Simulated Annealing to the HEN synthesis problem, as proposed by Dolan et al. (1989,90), will be discussed. First an introduction to the Simulated Annealing algorithm will be given (extracted from Nielsen 1994). This will be followed by a discussion of the convergence criteria and how to measure the value of the method. Finally Dolan et al's proposal will be outlined and discussed.

5.1 Introduction to Simulated Annealing.

Optimising an engineering system is - generally speaking - a complex task. A high number of continuous and discrete variables are often necessary in order to describe the system in a sufficient way. The mixture of continuous and discrete variables makes it rather difficult to perform a computer-aided optimisation of the system. The purpose of this section is to describe a rather new technique for optimising such systems. A method that seems to be well suited for a wide range of engineering problems. Although the method is based on rather complicated mathematics the basic idea and strategy is easily understood and the implementation of the method is almost straightforward.

The method described is called "Simulated Annealing" and has in the last few years received much attention. The method has been applied to a wide range of problems including: Design of integrated circuits (Kirkpatrick et al., 1983), Image analysis (Geman and Geman, 1984), Training of neural networks (Ackley et al.,1985), Floor planning (Otten, 1988), Batch-process scheduling (Das et al., 1990) and Design of heat exchanger networks (Dolan et al., 1990). It is not the intention to give a thorough review of the mathematics involved. Rather a short introduction to the main principles of the method is given.

The central issue in an optimising assignment is - from a given state - to find a better and if possible an optimum state. As an illustrative example for describing the procedure in Simulated Annealing, we consider a mountainous landscape where we are standing at a random point. Our task is to find the deepest valley in the area. The most logical way is to head downhill by the rule of steepest descent. If we follow that strategy we will soon find a valley where any immediate adjacent points are at higher elevation. We have found a minimum, but we have no way to be sure that this is the deepest valley in the whole area. There might be a deeper valley on the other side of a mountain range. This indicates that if our goal is to find a global optimum we must allow ourselves temporarily to move uphill in order to get to a deeper valley.

In contrast to most other optimising strategies Simulated Annealing allows us to move uphill. When we follow the strategy given by Simulated Annealing we will take

a step in a random direction. If the step is downhill we will accept it. If it is uphill we may accept it. The "may" is actually the most important feature in Simulated Annealing. In practice this "may" means that there is a probability **p** that the step is accepted. If the step is downhill the probability **p** is 1. If the step uphill is lifting us **Δh**, the probability **p** of accepting the step is

$$p = e^{-\frac{\Delta h}{\beta}} \tag{5.1.1}$$

The parameter β determines how steep we are allowed to move upwards. With a high value of β the possibility of moving upward is high while a near zero value of β means that all attempts to move upwards will be rejected. While decreasing the value of β we are able to make a search that initially allows us to move out of local minima and finally to a global minimum. With a sufficiently high starting value of β and a sufficiently slowly decreasing scheduling, the algorithm will lead us to an optimum or near-optimum state. It has been proven mathematically that the probability of finding an optimum state converge towards unity as the starting value of β is sufficiently large and the decreasing schedule is sufficiently slow (Laarhoven and Aarts, 1987).

The overall procedure when using Simulated Annealing can be shown in this pseudo-Pascal code:

```
Begin
    Initialise β
    Initialise starting point
    Calculate objective value of starting point
    Repeat
        Repeat
            Make a random step
            Calculate difference in objective function (Δh)
            If downhill then accept step
            If uphill then "maybe" accept step ( prob=exp(Δh/β))
        until sufficient move
        Decrease β ( β_new = β_old · α)  ( 0 < α < 1)
    Until β is sufficiently small
End.
```

This pseudo code is actually all the optimision related programming needed. Therefore the main task - when using Simulated Annealing - is to describe the system involved in a way that allows us to make random changes in the system. When the system is well described we have to experiment to find good values of β and α.

A computer program that optimises the function $f(x) = x^2(1+\sin(x)/2)$ is given in by Nielsen (1993). As shown in Figure 5.1.1, this function has a large number of local minimums. The code, that consists of less than 100 lines, shows the simplicity of the

implementation work. When optimising another function (or set of functions), simply change the objective function and the transition procedure.

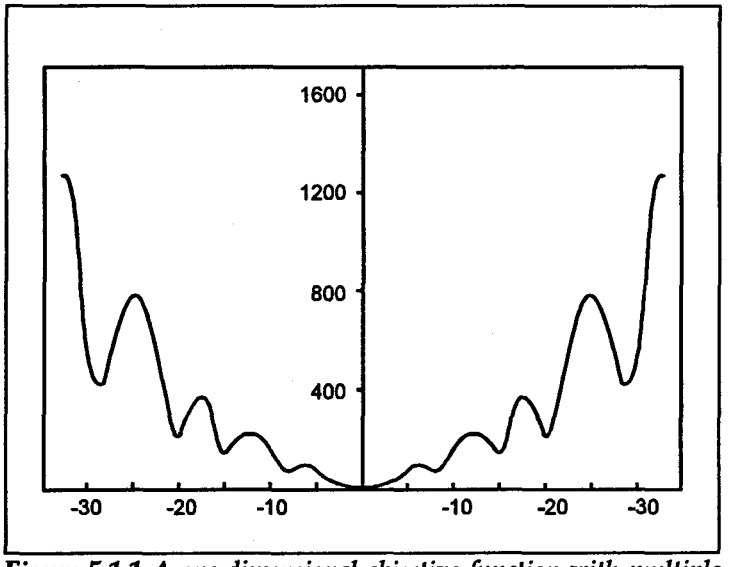


Figure 5.1.1 A one dimensional objective function with multiple local minimums. A computer code for optimising this function is given in Nielsen (1993).

When running the code for this example with different optimisation parameters (Initial value of β, α) it is noticed that the quality of the solution is dependent on these parameters. If it is important that the solution is a true global optimum, the optimisation parameters must be adjusted such that the initial value of β is very high and the decreasing schedule is very slow (α near 1). In most engineering cases, however, the objective function is based on predicted costs whose uncertainties must be considered. Therefore, usually a near optimum solution is sufficient. With the example in figure 2, every solution in the range of $-3 < x < 3$ are probably equally good.

The implementation work, based on Simulated Annealing, can be split into three parts

1. Define objective function
2. Define possible moves
3. Adjust optimisation parameters

Thus the major part of the optimisation assignment is to describe the physical behaviour of the system and only a little effort is needed for implementation of the optimisation routines.

5.1.1 Mathematical issues.

Although we do not want to go deeply into the details, some mathematical insight might be useful when building new applications. When using the Simulated Annealing algorithm, we continuously attempt to transform the current configuration into another configuration in the immediate neighbourhood. The outcome of every attempt only depends on the previous configuration. This is mathematically known as a Markov Chain. It is important though that the transition algorithm is capable of

reaching every possible state in the solution area. One of the main considerations is to allow the transition algorithm to move backwards.

5.1.2 The travelling salesman problem.

The Travelling Salesman Problem (TSP) is an often used example for global optimisation because it belongs to a class of minimisation problems for which the objective function has many local minima (Press et al., 1989). In short the Travelling Salesman Problem is to find the shortest route in which a salesman can visit a given number of cities. The steps of setting up the poblem for Simulated Annealing is simillar to the previous example. First it is necessary to define the objective function. In this case the objective simply is to find the shortest route in which n cities are visited. Therefore, the objective function can be given as

$$\sum_{j=1}^{n}\sqrt{(x_j-x_{j+1})^2-(y_j-y_{j+1})^2} \qquad (5.1.2$$

where each city is given by its coordinate (x,y). From the n'th city we return to the starting city $[(x_{n+1},y_{n+1}) = (x_1,y_1)]$. The next step is to define our transition procedure. A simple way to rearrange the route is simply to switch the order in which two cities are visited. With these short descriptions of the objective function and the transition procedure, it is easy to rebuild the computer code for this application. A more efficient set of moves is to remove a section of cities and place the section along another part of the route. A complete computer code using this rearrangement strategy is given by Press et al. (1989).

5.2 Criteria for convergence.

An extensive review of Simulated Annealing is given by Laarhoven and Aarts (1987). They cover the mathematical behaviour of the algorithm including convergence criteria and relation with statistical physics. They further discuss different cooling schedules and stop criteria.

The primary objective of this thesis is, however, not to dwell to long at the mathematics. Although some insight is useful and necessary the method will be judged by the real life performance rather than by theoretical convergence criteria.

Some highlights from the above reference (Laarhoven and Aarts, 1987) will be presented to introduce the general criteria for asymptotic convergence. A necessary condition (but not sufficient) for asymptotic convergence is that each individual Markov chain is of infinite length and that the control parameter (β or annealing temperature in the analogy) asymptotically goes toward 0. By applying some additional conditions Laarhoven and Aarts (1987) proves asymptotic convergence.

For any practical implementation, however, it will not be possible to find global optimum with probability 1. This is due to among others the finite length of the Markov Chain. For practical implementation Laarhoven and Aarts propose some general guidelines.

Initial value of control parameter (Initial annealing temperature):

This value should be high enough to allow virtually all transitions.

Stop critiria:

Either a fixed minimum value of the annealing temperature or when the changes in objective functions become sufficiently small.

Markov length:

This value can either be fixed or proportional to the number of variables.

Decrement in control parameter (Cooling schedule):

In general two classes of cooling schedules are proposed. The first is based on exponential cooling $T_{sa,i+1} = \alpha\ T_{sa,1}$ while the other is based on calculation of the standard deviation for each Markov chain.

Further the formulation of the problem must be such that every configuration is reachable from any point in a finite number of steps,

5.3 Simulated Annealing for HEN synthesis.

Dolan et al. (1989,90) propose a new approach to the HEN synthesis problem based on a tailored Simulated Annealing algorithm and a new superstructure framework. Since much of the work presented in the subsequent chapters rely heavily on the concept developed by Dolan et al., their approach will be described thoroughly.

5.3.1 Data structure

The first step in Dolan et al's approach is to define a new data structure for the heat exchanger network. The new data structure arises from the Grid diagram representation (Figure 5.3.1). Dolan *et al.* views the graph as a directed graph, where each side of the exchanger is treated as a node and the stream connections as pointers. Every node has three pointers that are directed towards other nodes. The pointers are used for information flows and can thus be used in recursive procedures. They use the pointer structure for downstream calculations. With e.g. a change in heat load for a single exchanger it is possible to trace the effect by calculating the results downstream from the affected exchanger. It is thus possible just to calculate the part of the network that has been affected.

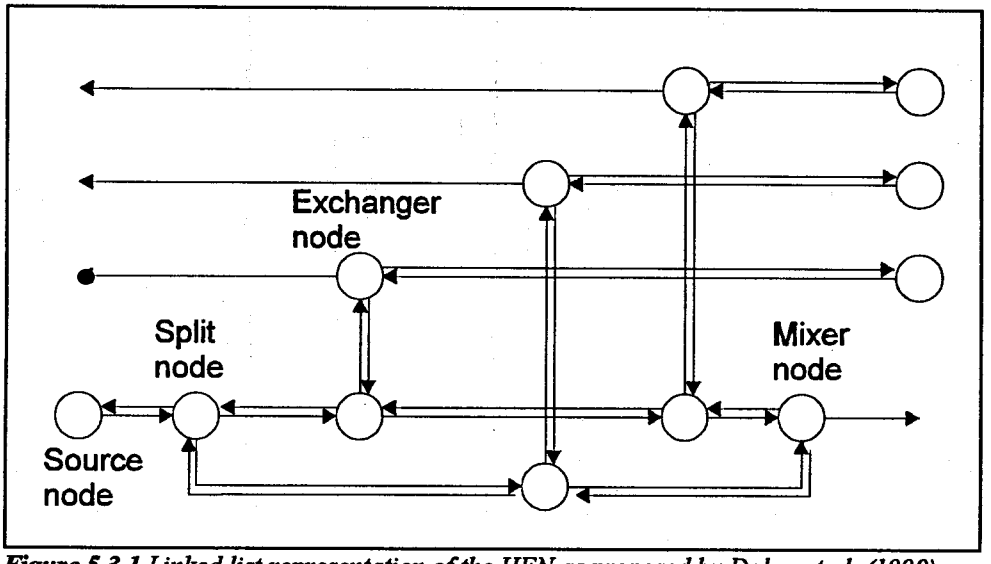


Figure 5.3.1 Linked list representation of the HEN as proposed by Dolan et al. (1990).

The pointers are directed such that one points downstream (*next*), one upstream (*previous*) and one toward the other side of the exchanger (*other*). Dolan et al. also allow splits in their network. For split nodes the *other* pointer is directed towards the next node along the split stream. And likewise is the *other* node of the combine node directed toward the previous node along the split stream. Each node is a variant record that contains specific information on the node.

For each change in the network, calculation is done in three steps: (i) material balances; (ii) energy balances; (iii) area sizing. The node contains the necessary information for calculations.

In the first step the heat capacity flow rate (F) distribution is calculated by tracing along the *next* pointers. When a split is reached the pointers *next* and *other* are traced out. The first time a combiner is reached a boolean flag is set true and tracing is stopped. The second time it is reached the flag is set false and tracing continues.

In the next step when F is fixed, the energy balances are calculated. The resulting outlet temperature from each heat exchanger node is calculated by $T_{out}=T_{in}+q/F$ where q is the heat exchanger load. The tracing is done in the same way as for mass balances.

Finally in the third step when all temperatures are available, the heat exchanger areas can be calculated in a similar way. Again the necessary information is available in the heat exchanger nodes. During the area calculation it is checked whether a minimum approach temperature is satisfied. If not, the cost is set to infinity and the move is rejected.

5.3.2 Move sets.

Dolan et al. (1990) employs six different moves.

> *Add exchanger*: A new exchanger (two exchanger nodes) is added randomly in the network. The heat load is chosen as a random fraction of the minimum utility

need from the two streams. After the exchanger is inserted, the energy and design equation are calculated along with the resulting change in objective function (ΔC).

Delete exchanger: A random exchanger in the network is selected and deleted. All affected nodes are then recalculated.

Change q: A random exchanger is selected and the heat load (q) is changed. The maximum change in q is 20 % of the current heat load.

Shift q: Shifting heat load between two exchangers on the same randomly chosen stream. The maximum amount of heat shifted is set to 40 % of the minimum of the two heat loads.

Add split and exchanger: Adding a split and combiner with a new exchanger on the split stream.

Change split ratio: Changing the split ratio for a random splitnode with a random fraction between -0.2 and 0.2. Split ratios greater than unity or less than zero are set to unity or zero respectively.

A split is deleted when there is no exchanger on a split.

Under perfect conditions Simulated Annealing demands that the probability of attempting a step should be the same as the probability to attempt the reverse step. This symmetry is fulfilled regarding adding and deleting exchangers, changing and shifting heat loads and changing split ratios. Adding and deleting splits, however, are asymmetric since the probability for attempting to add a split is somehow higher than the probability of attempting to remove a split (1/6 for attempt to add split, less than 1/6 for attempt to remove split since not all exchanger removal causes an empty split). Dolan et al. pointed out that this slight asymmetry does not seem to affect the performance of the algorithm.

Dolan et al. investigates two different cooling schedules. The first is the exponential cooling schedule originally proposed by Kirkpatrick et al. (1983)

$$T_{sa,i+1} = \alpha\, T_{sa,i} \tag{5.3.1}$$

where α is a constant between zero and unity

The second is the one proposed by Aarts and Larhoven (1985)

$$T_{sa,i+1} = \frac{T_{sa}}{\ln(1+\delta)\, T_{sa,i} / 3\sigma_i + 1} \tag{5.3.2}$$

where σ_i is the standard deviation of the cost at the current annealing temperature and δ is a parameter that controls the speed of the simulated annealing procedure. The second cooling schedule is an attempt to keep a constant distance from the equilibrium point.

Further Dolan et al. discuss selection of the Markov length based on the observation by Aarts and Laarhoven (1985). They found that the theoretical length should be in excess of 6000 moves for a seven stream problem. Based on experiments they later

reduced the number of moves to around 400 moves and found that the length in general should roughly scale with the square of the number of streams. It should be noted here that there is a close relationship between cooling schedule and Markov length. With long Markov length a faster cooling schedule can be applied than for a short Markov length.

A reasonable value of the initial temperature was found by experiments while the stopping criterion was a fixed value for the annealing temperature.

The proposed algorithm was applied to a well-studied example problem from Floudas et al. (1986) for which Dolan et al. (1990) found a new low cost solution.

They further tested the same problem applying a stepwise price function for heat exchangers to represent off the shelf heat exchanger units. They concluded here that the algorithm was unaffected by these discontinuities.

It is the latter observation that seems to be the most promising element of Dolan et al's work. The advantage of Simulated Annealing is that it is derivative free and thus does not suffer from numerical difficulties when including nonconvex and/or discontinuous expressions in the constraints or in the objective function. The major disadvantage inherent in the algorithm is the computational expense. This expense is principally due to the random search. Lots of effort, especially in the beginning of the search, are wasted by searching in inferior areas.

From a practical view, however, the advantages look so promising that it overshadows the computational inefficiency of the algorithm.

6
IMPROVED OPTIMISATION FRAMEWORK FOR THE HEAT EXCHANGER NETWORK DESIGN

In this chapter an improved framework for heat exchanger network synthesis is presented. The proposed framework addresses itself to the synthesis of practical industrial heat exchanger network - grassroot as well as retrofit design. The framework accounts for non-constant heat capacities and heat transfer coefficients, detailed heat exchanger modelling, flexibility and pressure drop considerations. Which are all important issues that so far have not been sufficiently addressed in the literature.

The key element for obtaining this kind of framework is to treat each element of the HEN from a conceptual point of view. Each element is described by its functional behaviour. From the conceptual description a set of generic elements describing the general functions of the network is derived.

In practice, the network is split into two categories representing the thermodynamic properties (Process Streams) and the physical properties (HEN nodes) respectively.

The new representation is based on an extended version of Dolan et al's linked list representation. In the extended version each element is treated as an individual object using an object oriented approach. By deriving all network elements from a common base of generic units the new framework can handle models of different complexity in a consistent way. The simulated annealing algorithm is adopted for optimising the resulting HEN synthesis problem. The object oriented representation combined with the Simulated Annealing algorithm allows for synthesis of problems with a high degree of complexity and thus the kind of problem met in the industrial practice.

6.1 Introduction.

Heat exchanger network (HEN) design is a discipline of industrial significance. The heat exchanger network is the link between the core process and the utility system and is thus - to a large extend - responsible for the overall energy demand in a process plant. This is one of the reasons why HEN design has become one of the most studied synthesis problems in chemical engineering. The area has been reviewed several times in the last 25 years (e.g. Nishida 1981, Gundersen and Naess 1988, Grossmann 1992). The extensive review by Gundersen and Naess (1988) outline the most significant steps in the history of HEN synthesis. Later Grossmann (1992) has outlined the latest development within HEN synthesis.

Being a part of a total synthesis problem HEN synthesis cannot be viewed isolated. Gundersen and Naess (1988) mention that due to the interaction between the HEN and the process and utility system some stream parameters can be viewed as "hard" and some can be viewed as "soft" parameters. Further some qualitative aspects such as flexibility, operability and controllability are very important in the final design selection but are yet difficult to handle at the early design stage.

All reported HEN synthesis methods operate with hot and cold process streams. These streams are then matched with heat exchangers in order to optimise the total cost in terms of an economic evaluation base (e.g. net present value). The streams arise from the total processing system and are thus not necessarily independent of the degree of heat recovery in the final heat exchanger network. This is partly due to the fact that some components in the heat recovery system are active (i.e., changing with changing conditions). A typical active component is an integrated compressor where the inlet stream is cooled. The temperature of the outlet stream is dependent of the compressor inlet temperature.

6.2 Generic HEN components.

In this section the elements of the heat exchanger network will be treated in a systematic way discussing the nature of each element. The purpose is to define a general representation of the basic network element features with extensions in mind.

The elements of the HEN can be grouped into two basic categories:

1. Process Streams
2. Heat exchanger network units

The two categories will be discussed in view of their functional behaviour.

Process streams:

Traditionally HEN synthesis has been based on optimal configuration of heat exchangers placed between a set of hot process streams and a set of cold process streams. Each of these process streams were defined by an initial temperature, a target temperature, a heat capacity flow rate and a heat transfer coefficient. For many industrial processes however this process stream definition is too narrow. It is therefore necessary to look at the conceptual role of a process stream to understand the general process stream behaviour.

A process stream is the mean for mass and energy transfer between parts of the process plant. A process stream can basically originate from the surroundings or from a unit operation. The target of the process stream is similar - either another unit operation or the surroundings. The initial state of the process stream is obviously dependent on the unit operation from which it originates or alternatively the surroundings. The target state of the process stream is dependent on the target unit operation that in turns could be dependent on the optimised state. These dependencies

will initially split the process streams into two groups - *fixed process streams*, where inlet and outlet conditions are process determined and thus available a priori and *non fixed process streams*, where the inlet and outlet conditions are not fully determined a priori. To clarify the meaning of non fixed process streams, two examples will be given. The first example is cooling of discharged gas (stack gas), where the initial state is fixed (temperature and flowrate) while the final temperature is dependent on the amount of heat needed by the other process streams which in turn is an economical trade off. This means that the optimum outlet temperature is dependent on the final optimised solution. The second example is steam rising in highly exothermic processes. The optimum amount of steam produced in the process is again dependent of the optimised HEN. A certain class of non fixed process streams is *bounded streams*. As the name suggests, bounded streams are non fixed process streams where inlet and outlet conditions are constrained to lie within a certain range.

Another way of grouping the process streams is, whether the streams are *constant property process streams* or *variable property process streams*. For constant property process streams the thermodynamic properties (for example heat capacity and heat transfer coefficient) for the process stream will be assumed constant, while for variable property process stream these properties will vary with temperature and/or pressure. The assumption of constant property values can be a reasonable approximation for a long range of pure substances with no phase changes. However fully or partial phase changes are very common in general process synthesis and must therefore be taken into account. A compromise between the constant and variable property process streams is the *piecewise linearised property process stream*, where the variation in property changes can be handled by piecewise linearisation. An example of variable and linearised property streams are cooling of humid air to under the dew point, where the assumption of constant property can be fatal. This case is outlined in figure 6.2.1a where the heat content of humid air is shown as a function of the temperature. In fig. 6.2.1b the heat content based on a constant property assumption is outlined. Now if a heat exchanger is designed to change heat between the humid air and water, with a minimum temperature difference ΔT_{min}, the heat exchanger may be designed too small or even infeasible. Besides the changes in heat capacity the heat transfer coefficient also changes dramatically under condensation.

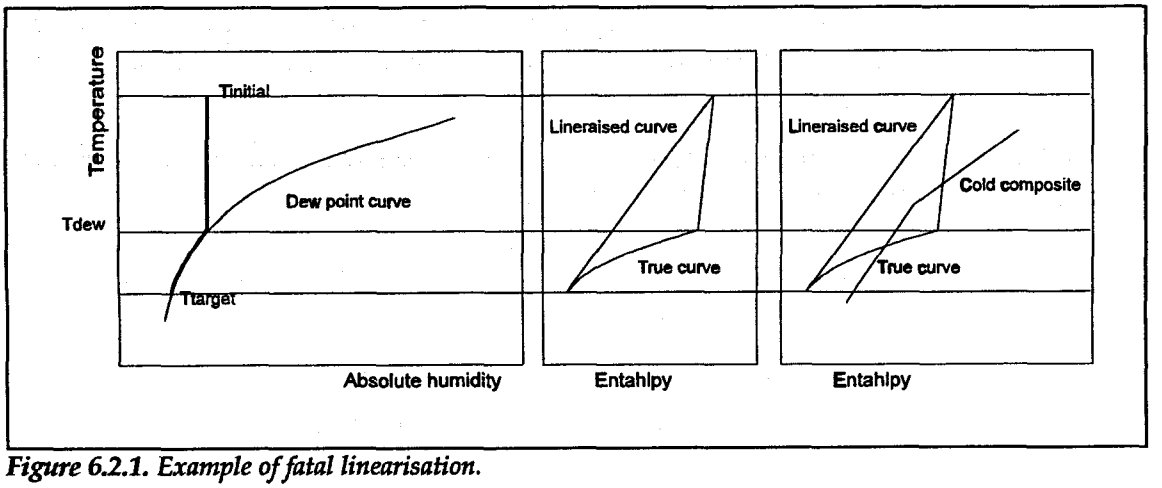


Figure 6.2.1. Example of fatal linearisation.

It is not only for partial and fully phase changing streams that have to be described as a variable or a piecewise linearised stream. Other examples of variable streams are continuously reactive streams such as oxidation processes (for example. NO to NO_2 oxidisation in nitric acid plants), where reactions take place along the streams.

It is possible to put these elements into a general stream hierarchy. As base in the stream hierarchy is a generic stream object. From this generalised stream object a tree of different models is derived. Traversing down the tree there is an increase in model complexity. An example of a stream model hierarchy is outlined in figure 6.2.2.

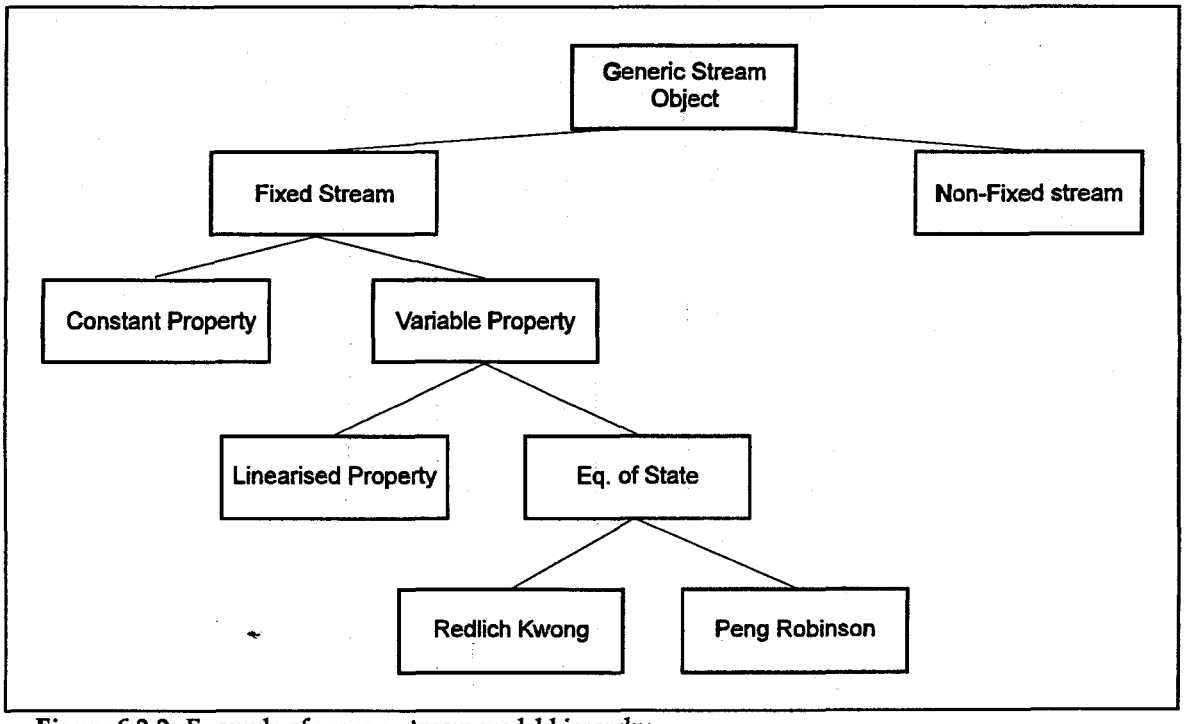


Figure 6.2.2. Example of process stream model hierarchy.

While most HEN synthesis approaches are based on the fixed constant property process stream definition, a typical industrial process plant has several other process stream types. The non fixed streams are normally handled in an iterative way, where the non fixed streams initially are assigned a target temperature, whereafter the fixed streams HEN synthesis problem is solved. Finally the non fixed process streams target temperatures are updated.

With the proposed hierarchical description of the process stream it is also possible to define streams with uncertainty range.

Network nodes:

Heat exchangers in HEN are the means for exchanging heat from the heat releasing streams to the heat demanding streams. In general a HEN synthesis procedure must be able to handle new as well as existing heat exchangers. In HEN synthesis studies the optimisation variables are typically the heat load Q. With a given heat load the resulting temperatures can be calculated and subsequently the physical size of the heat

exchanger can be calculated. The physical size, often represented by the heat transfer area A, depends on the type of exchanger. The minimum heat exchanger area for a given heat load and given temperatures is obtained when heat transfer is counter currently. However, most industrial heat exchangers are not truly countercurrent. The sizes of these exchanger types are often calculated using correction factors.

Splitters and combiners are two other elements in a basic HEN. In several cases splitting a process stream can give some advantages in heat transferring. This is normally the case when the process plant consists of one heat releasing stream and several heat demanding streams. Since most streams have a specific target these must be mixed again, which is done in combiners.

The Heat and mass flow distribution are thus governed by the heat exchangers, splitters and combiners.

A special subgroup of HEN nodes is the *Utility nodes*. The utilities are the means for importing/exporting energy from the HEN to fulfil the stream constraints. Thus utilities to a large extend represents the operational costs of the HEN.

The last group of units that belong to the network units is the auxiliary nodes. These auxiliary nodes can be pumps, compressors, control valves etc., that are necessary for the HEN to function.

As for streams, it is possible to build an object hierarchy for HEN units. All units are derived from a generic unit model. From that other units are derived in increasing order of complexity. An example of a HEN unit model hierarchy is outlined in figure 6.2.3.

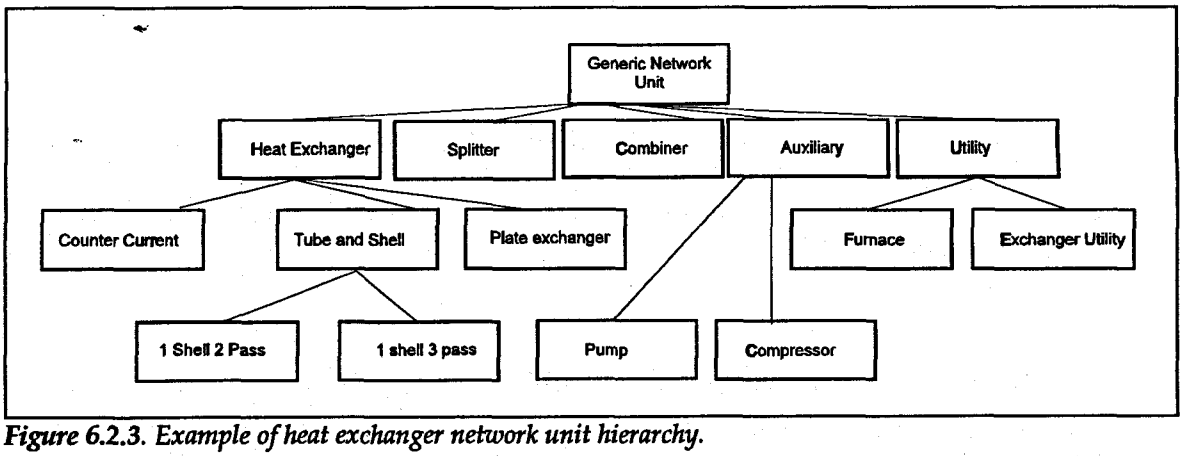


Figure 6.2.3. Example of heat exchanger network unit hierarchy.

To represent the network the grid diagram originally proposed by Linnhoff and Flower (1978) is used. The grid diagram (Linnhoff and Flowers 1978) is perfectly suited to illustrate the functional behaviour of the two basic elements in the HEN. In Figure 6.2.4 a HEN is shown with different elements.

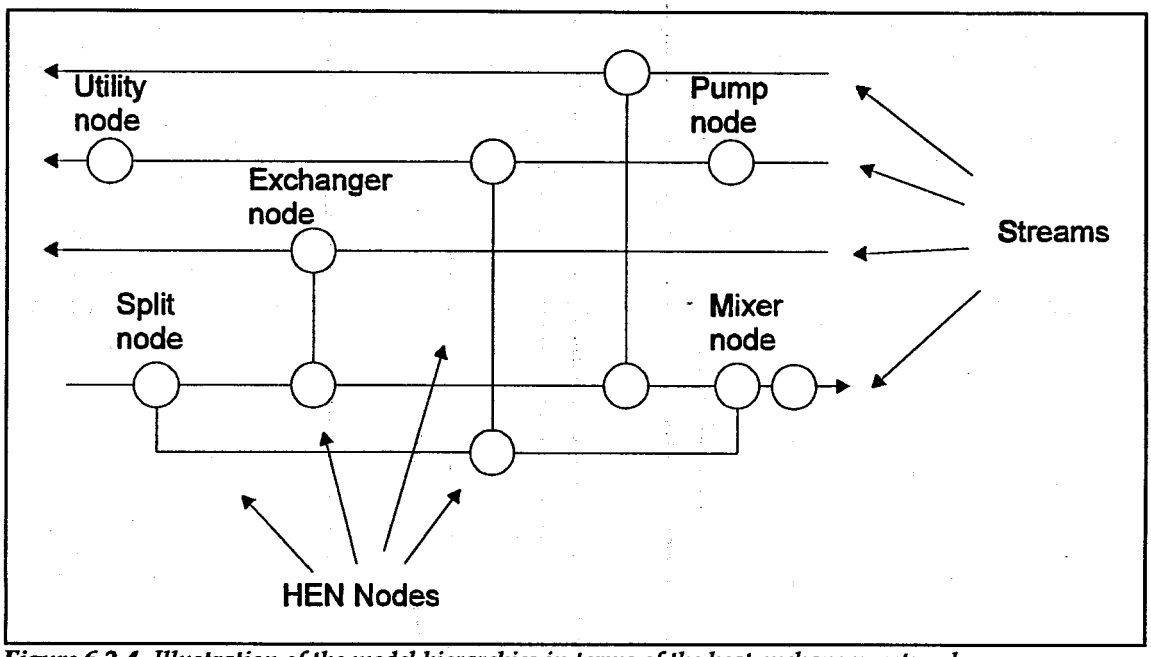


Figure 6.2.4. Illustration of the model hierarchies in terms of the heat exchanger network.

6.3 Modelling in view of the Generic Representation.

HEN elements can be viewed in hierarchically as shown in figure 6.2.3. From a Generic base for each of the four elementary groups, increasingly detailed models can be derived. The new element in this approach is that the network calculations do not follow a global specification. In the proposed framework the calculations are node specific respectively stream specific. A comparison between the traditional approach and the functional approach proposed here is given table 6.3.1. Instead of specifying general equations for energy balances and heat exchanger ratings the functional approach just uses a generic description of what is going on. The actual equation depends on actual nodes and actual streams that are involved. An example using a piecewise linearised stream model together with a countercurrent heat exchanger model is shown in table 6.2.

6.4 Data representation of the heat exchanger network.

An important element in implementing a framework which is sufficient for industrial HEN synthesis is the data representation. A good programming practice is to make the data structure reflect the problem and not vice versa. In this case the data representation must be able to handle multiple process stream types, multiple heat exchanger types. More importantly, the data representation must be able to handle structural changes in the HEN.

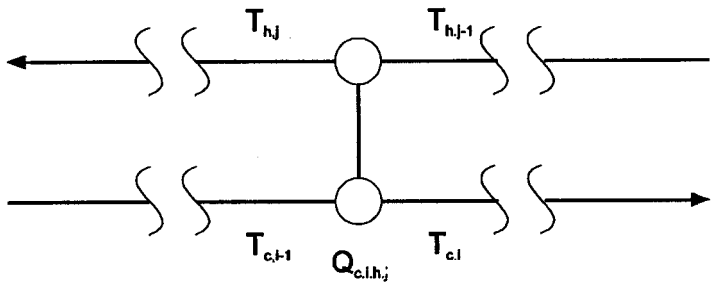
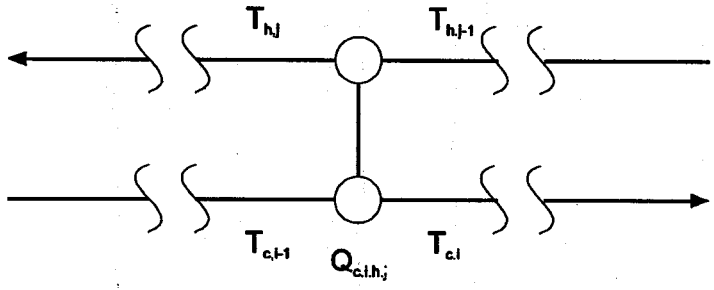
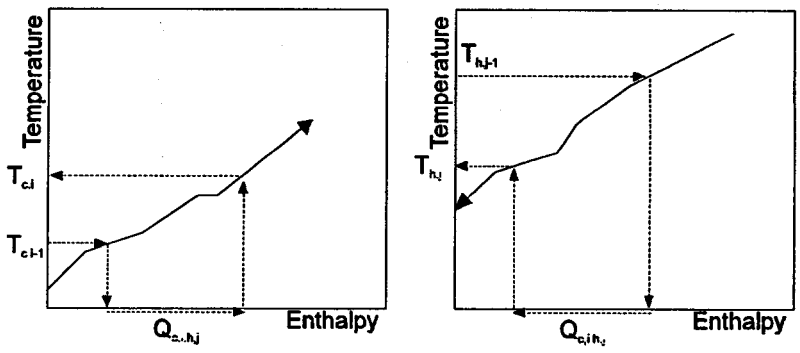
<table>
<tr><th colspan="2">Network modellling</th></tr>
<tr><td colspan="2"> 
</td></tr>
<tr><th>Traditional approach</th><th>General approach</th></tr>
<tr><td>Temperature calculation
$$T_{c,i} = T_{c,i-1} + \frac{Q_{c,i,h,j}}{CP_c}$$
$$T_{h,j} = T_{h,j-1} + \frac{Q_{c,i,h,j}}{CP_h}$$
Equipment size calculation
$$A_{c,i,h,j} = \frac{Q_{c,i,h,j}}{\Delta T_{\ln,c,i,h,j} \cdot U_{c,h}}$$
where
$$\Delta T_{lm,c,i,h,j} = \frac{\left(T_{h,j-1} - T_{c,i}\right) - \left(T_{h,j} - T_{c,i-1}\right)}{\ln\left(\frac{\left(T_{h,j-1} - T_{c,i}\right)}{\left(T_{h,j} - T_{c,i-1}\right)}\right)}$$
and
$$\frac{1}{U_{c,h}} = \frac{1}{h_c} + \frac{1}{h_h}$$</td><td>Temperature calculation
$$T_{c,i} = F\left(T_{c,i-1}, Q_{c,i,h,j}, \dot{m}\right)$$
$$T_{h,j} = F\left(T_{h,j-1}, Q_{c,i,h,j}, \dot{m}\right)$$
Equipment size calculation
$$A_{c,i,h,j} = \int_0^{Q_{c,i,h,j}} \frac{1}{U_{c,h}\,\Delta T} dQ$$
where
$$U_{c,h} = F\left(h_c, h_h\right)$$
and
$$h = F(T)$$</td></tr>
</table>

***Table 6.1** Comparison between the traditional approach and the general functional approach.*

Network Modelling



Piecewise linearised properties
Counter current heat exchange

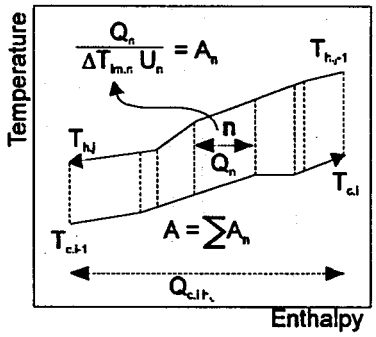


Temperature calculations

$$T_{c,i} = F\left(T_{c,i-1}, Q_{c,i,h,j}, \dot{m}\right)$$

$$T_{h,j} = F\left(T_{h,j-1}, Q_{c,i,h,j}, \dot{m}\right)$$

Equipment size calculation



$$A_{c,i,h,j} = \sum\left(\frac{Q_n}{\Delta T_{lm,n} U_n}\right)$$

6.4.1 Object oriented approach

The above demands for the data representation seem to be most flexibly handled using an object oriented approach (OOA). Object orientation in a system representation is characterised by two key features:

1. Encapsulation or abstraction
2. Inheritance

The idea of encapsulation is that encapsulations should be complete in that they include all the essential properties of an item. In programming terms this means that objects should encapsulate both data and procedures. This reflects the thought that objects should represent essential features without including the background.

Inheritance on the other hand describes the way structural relationships between objects are handled. The idea of inheritance is to avoid storing the same data or procedure more than necessary. The relationship between different similar objects is stored in an object hierarchy. Inheritance is the ability to deal with generalisation and specialisation. Subobjects inherit data and methods from its ancestor and may add others or override those inherited. The object hierarchy can thus be used to represent different levels of complexity of elements in the system modelling.

For heat exchanger networks there are two conceptual elements that can readily be represented in object hierarchies. These object hierarchies will be

- Process stream object hierarchy
- Network node object hierarchies

The process stream objects contain data and methods for property calculation for each process stream. The network node objects contain data and methods for the units in the heat exchanger network. In the following the necessary data and methods for process stream and network node objects will be outlined.

6.4.2 Process stream objects

A process stream object contains the thermodynamic properties of the process stream. These properties can be used to calculate other thermodynamic properties. A typical example is a method that calculates the specific enthalpy as a function of the temperature.

For network calculations the process streams must hold at least two methods:

1. Calc_H(T,H0) : Calculation of enthalpy as function of temperature
2. Calc_T(H,T0) : Calculation of temperature as function of enthalpy

The generic process stream object (TGenericStream) is defined as

```
Class(TObject)                  {General object}
      Name            :         String  {stream name}
      Tinitial        :         Real    {Initial stream temperature}
```

```
        Ttarget :       Real    {Target stream temperature}
        MassFlow        :       Real    {Stream mass flow rate kg/s}
        Constructor     Init
        .
        .
        Function        Calc_H(T,H0): Real{ void for the generic object}
        Function        Calc_T(H,T0): Real { void for the generic object}
End
```

For a simple process stream with constant properties the object header is:

```
Class(TGenericStream)                   { Inherited from Generic stream}
        Cp      :       Real                    { Heat Capacity kJ/Kg/K}
        h       :       Real                    { Film transfer coefficient}
        Constructor     Init
        .
        .
        Function        Calc_H(T): Real { overwrite ancestors' method}
        Function        Calc_T(H): Real { overwrite ancestors' method}
End
```

For the constant property stream the methods will be as

```
Calc_H(T,H0) = (Tinitial-T)*MassFlow*Cp-H0
Calc_T(H,T0) = T0-H/MassFlow/Cp
```

where H refers to the enthalpy (based upon H=0 at T=Tinitial).

More complicated calculation can be carried out if going down through the object tree. The important feature in OOA is, that is possible to extend the model in small steps reusing the full capability of the previous model.

6.4.3 Network node objects

Network nodes contain the physical characteristics of the different elements in the heat exchanger network. These elements are traditionally heat exchangers, splits and mixers but could also be valves, pumps, compressors, turbines etc. The network node objects contain data and methods that relate the inlet condition to the outlet condition. In the calculation of this input-output relation, use is made of the specific process stream object. Further, data and methods for sizing (design equations) must be available and finally methods for cost estimation used in the objective function.

For all network node objects there most be methods and data that can calculate the output condition given the input condition.

```
Calc_Output(Input)
```

and further a method to calculate the cost of the given operation

```
Calc_Node_cost
```

Again the methods can be derived starting with simple model and then gradually increase the complexity.

6.4.4 Linked list representation of objects.

Dolan et al. (1990) proposed a linked list to represent the structure of the heat exchanger network (Figure 5.3.1). The data structure treats each side of a heat exchanger as a network node. The heat exchanger node has a pointer to the other side of the node as well as to the downstream and upstream nodes. Splitters and mixers are also represented as nodes. Each node is represented by a variant record. Dolan et al. use the linked list representation to perform downstream calculations and thus only calculate changes in the affected part of the network. The linked list representation also allows for convenient handling of structural changes and keeps the necessary computer storage down to a minimum.

The linked list representation is adopted in this work but instead of representing each node as a variant record a more general approach using objects is applied. The network nodes in this work contain the same directed pointers as Dolan et al. The nodes, however, contain more information. Generally all nodes have an associated process stream which is a pointer directed to the stream on which it is placed. It also has an associated *Price Function* that has methods for calculating the cost of the given operation. Finally it has the above mentioned method for input-output relations.

6.5 Implementation - *HEN Explorer.*

To illustrate the potential of the proposed framework *HEN Explorer* - a prototype Network Synthesis tool - is developed based on the conceptual idea given in this chapter. The program has been developed in the Object Pascal (Borland Pascal).

Implementation of the framework has been carried out with two keyproperties in mind:

- Extendibility
- Flexibility

The first property emphasises the wish to include further elements in the feature (for example, unit integration) while the second reflects the wish to be able to handle different levels of complexity in the same framework.

The object oriented approach has moved major programming work from the overall system to specific modelling. This means that the main program is limited by a range of calls to the objects representing the elements of the network. These elements then take care of the specifics.

6.5.1 Overview of program structure.

HEN Explorer is build around the hierarchies developed in chapter 6.2. It is, however, important to know how the HEN elements are interrelated. In *HEN Explorer* a new object is defined as *NodeStream* (TNodeStream). This object contains (owing in

Object Oriented vocabulary) a stream derived from the *Generic Stream Object* (TGenericStream) and a collection of exchangers, splits etc. that are derived from the *Generic HEN Object* (THenNode). Together with these elements (properties in OO) the *Nodestream Object* also contains methods. There are methods able to perform calculations on the *Nodestream* using properties and methods from the *Stream Object* and the *HEN Objects*. The *Nodestream Object* also has methods for inserting, moving and deleting *HEN Objects*.

The declaration of the *Nodestream Object* (TNodeStream) thus contains the following methods (among others)

```
Class(TObject)
      StreamProperties : TGenericStream; {Derived from Generic stream
      object}
      HENNodes         : TCollection;    {Collection of HEN Objects}
      .
      .
      .
      Constructor Init;
      Function InsertExchanger: Boolean; {Insert exchanger - returns true
               if  feasible}
      Function ChangeExchanger: Boolean; {Change heat load on specific
               exchanger}
      Function CalcMassFlows: Boolean; {calculate mass flow
distributions}
      Function CalcTemperatures: Boolean; {Calculate Temperature
               distributions}
      Function CalcNodeCosts(var Cost: real): Boolean; {Calculate Costs
               for HEN obj.}
      .
      .
end;
```

This representation allows for the flexible handling of different HEN models. It is thus possible to work with any combination of stream models and any composition of HEN node objects. The *Nodestream Object* just works on general terms using the specific models that are encapsulated in the objects it holds. For calculating temperatures and others the *Nodestream Object* calls the methods and properties encapsulated in its child objects.

To make the picture complete the *Nodestream* also has a parent object, which will be defined the *Network Object* (TNetwork) representing the complete heat exchanger network. The *Network Object* holds all the Nodestreams which in turn holds Process Streams and HEN nodes. An illustration of the overall ownership between object elements is given in Figure 6.5.1.

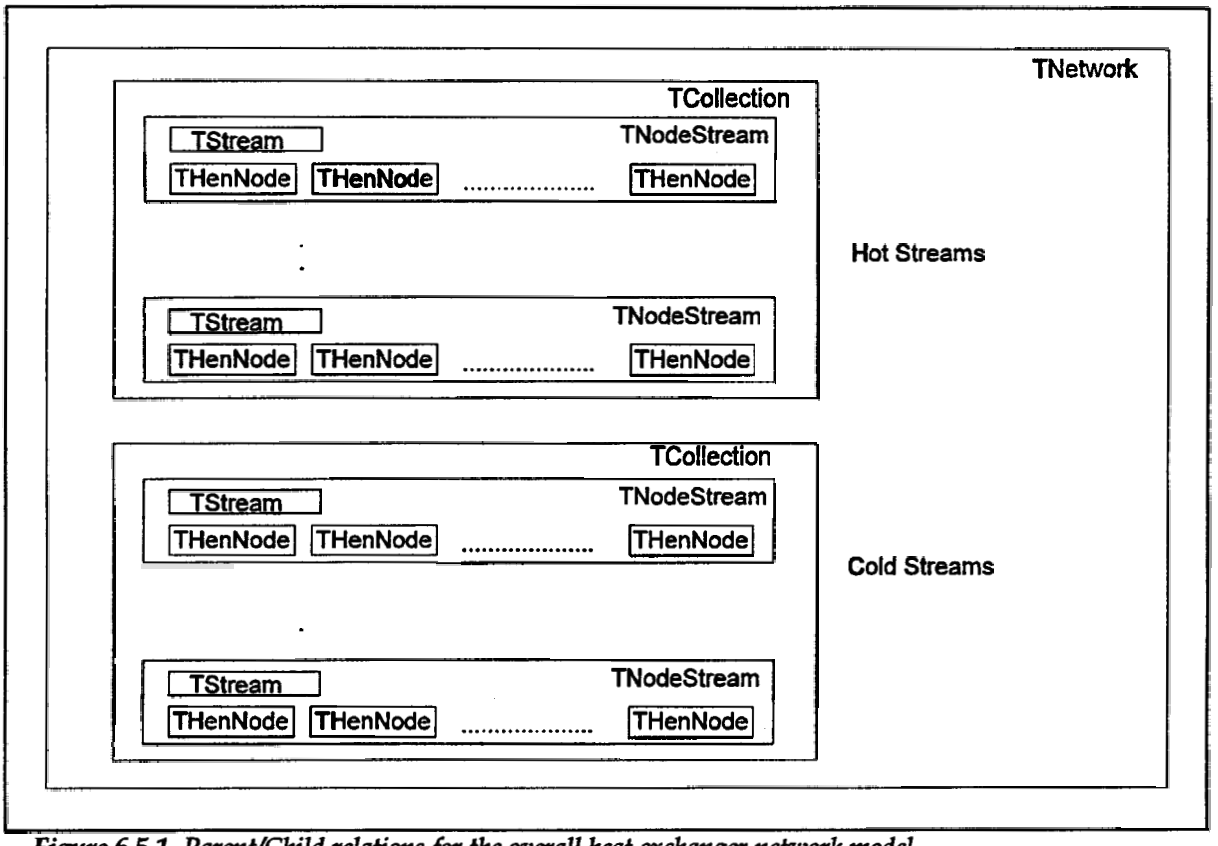


Figure 6.5.1. Parent/Child relations for the overall heat exchanger network model.

A very important element in the implementation work is the flow of information. In OOP every task is carried out using commands or orders. A parent object sends an order to one of it child that then carries out the order based on its encapsulated methods and returns if necessary the results to its parent (and maybe to other objects).

In *HEN Explorer* two ways of information flow is used. The first way is through parent/child relations. Every HEN node can thus call the property calculation models from its parent Nodestream which in turn call the methods from its stream object. The other way is through the pointer structure as proposed by Dolan et al. (1989,90) described in chapter 6.4.4. For heat exchanger calculation e.g. it is necessary to get information from the adjacent HEN node. Thus for area calculation the HEN node has access to its parents property methods and its adjacent node's parent property methods.

6.5.2 Process stream models.

Currently two practical process stream models derived from the process stream hierarchy are available in HEN Explorer

1. Constant property stream model
2. Piecewise linearised stream model

Constant property stream model:

The constant property stream model follows the "classical" formulation as outlined in table 6.1. Enthalpy changes are calculated directly by using a constant heat capacity.

Piecewise linearised stream model:

In the piecewise linearised stream, the stream is split in temperature intervals each with constant properties. Enthalpy changes are calculated by interpolation between the temperature intervals.

The piecewise linearised model can consist of any number of stream segments and is thus very flexible in use. Most practical problems can be linearised in a finite number of segments within reasonable accuracy. Normally no more than 5-6 intervals are necessary.

More complex models:

For most conventional problems the two stream models listed above are sufficient for stand alone optimisation of heat exchanger network. However, if the framework is implemented with a process simulator interface, then it will be desirable to be able to call the more accurate property methods in the simulators. The implementation of the generic stream model in HEN Explorer allows for this later enhancement. This enhancement could also include streams with associated reactor models etc.

6.5.3 HEN unit models.

Heat exchangers are available according to the object hierarchy in Figure 6.5.2. THexNode is a generic model that holds common features for all heat exchanger models. This includes heat load (Q) and heat exchanger area (A). THex_Count is an implementation of the counter current heat exchanger model. THex_1_2 is an implementation of a multipass 1-2 exchangers using the design methodology proposed by Ahmad et al. 1990. Two retrofit models are available at the moment: 1) TRetro_Hex_Count that is a retrofit version of the THex_Count model and 2) THex_Retro_1_2 is a retrofit model of THex_1_2. All heat exchanger node objects have an associated price function derived from a general price function object hierarchy.

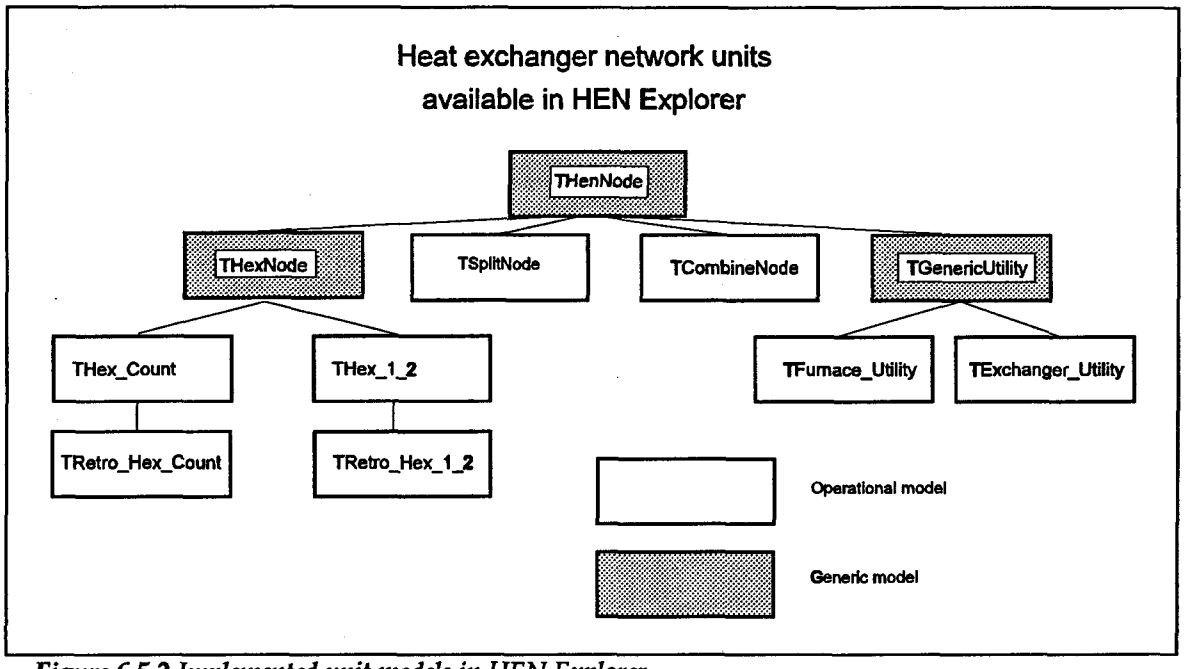


Figure 6.5.2 Implemented unit models in HEN Explorer.

Common features for all THexNodes:

As mentioned above all *THexNodes* have the fields Heat Load Q and Heat Exchange Area A. Further they all have the same Input-Output relations. For mass flow and energy balances this gives

```
MassFlowOut = MassFlowIn
Tout = ParentStream.Calc_T(Q,Tin)
```

The second line should be read as: Call the associated process stream to calculate the outlet temperature as a function of inlet temperature (Tin) and heat load (Q).

THex_Count model:

The *THex_Count* HEN node represents a truly countercurrent heat exchanger. The heat exchange area is calculated using the associated process streams property methods. Thus, for a constant property stream the heat exchange area is calculated as

$$A = Node.Q/U/DT_{lm}$$

where

```
1/U = 1/node.h + 1/node.other.h
```

and

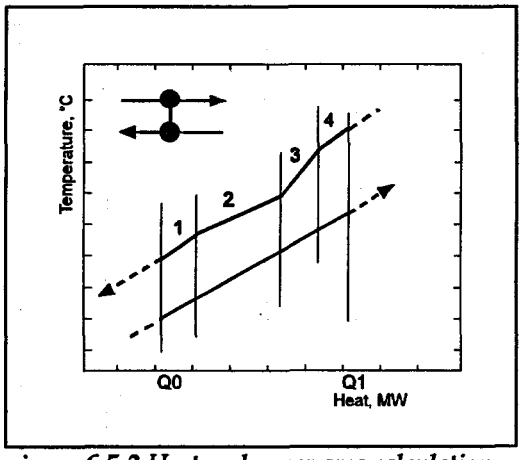
$$\Delta T_{lm} = ((node.Tin-node.other.Tout)-(node.Tout-node.other.Tin))/ \ln((node.Tin-node.other.Tout)/(node.Tout-node.other.Tin))$$

node represents the present side of the exchanger where *node.other* represent the other side of the exchanger. If both streams are not constant property streams, the calculations will be divided in intervals using the same equations for each interval ($A = \text{Sum } A_i$).

In practice all streams have a method called

```
MakeTQList(Tin, Tout, Massflow: Integer; List : TCollection)
```

A call to MakeTQList with specified input and output temperature and specified mass flow rates returns a list with properties for each enthalpy interval. An example with two different stream models is outlined in Figure 6.5.3. The hot stream is a piecewise linearised stream and the cold stream is a constant property stream. A call to MakeTQList for the hot stream returns a list with four elements representing the enthalpy intervals. A call to a constant property's MakeTQList will always return a simple list with only one element. Based on the two lists a third list can be established. Each interval in the third list has constant properties. In this case the interval boundaries are the same as for the hot stream alone since the cold stream has constant properties throughout the exchanger. Area calculation can then be performed using the ΔT_{lm} for each enthalpy interval.



igure 6.5.3 Heat exchanger area calculation n HEN Explorer.

Cost functions available for the counter current model are

```
Cost = C1 + C2 * Area                    {Linear cost function}
Cost = C1 + C2 * Area^C3                 {Exponential cost function}


          C1 + C2 Area   for Area<C5
Cost =                                   {Piecewise linear cost function}
          C3 + C4 Area   for Area >C5


Cost = C1 + C2*(Area/N)^C3
```

where N is calculated as the number of shells based on a maximum shell size (AMax).

Other price functions can easily be added when necessary.

THex_1_2 model:

The multipass 1-2 heat exchanger is derived from the counter current model. For calculation of heat exchange area a correction factor F_T is applied to the design equation (see chapter 3.7)

```
A = Node.Q/U/DTlm/FT
```

For a given number of shells the value of F_T can be expressed in terms of thermal efficiency P and capacity flow ratio R (see chapter 3.7 for definitions). An analytical expression for F_T can be derived (Ahmad 1985)

$$F_T = \frac{\sqrt{R^2+1}*\ln\left[\frac{(1-y)}{(1-RY)}\right]}{(R-1)*\ln\left[\frac{2-Y(R+1-\sqrt{R^2+1})}{2-Y(R+1+\sqrt{R^2+1})}\right]}$$

where

$$Y = \frac{1-\left(\frac{1-RP}{1-P}\right)^{\frac{1}{N}}}{R-\left(\frac{1-RP}{1-P}\right)^{\frac{1}{N}}}$$

where N is the number of shells in series.

Ahmad (1985) showed a simple method for selecting the number of shells based on an equidistance from infinite slope $X_P = (dF_T/dP)_{inf}$. This model is implemented in THex_1_2.

The calculation of number of shells and area follows the countercurrent model based on calls to MakeTQList for each stream. The heat exchange area and number of shells area are thus calculated for each enthalpy interval.

Practical reasons can also limit the maximum size of an individual shell. For that reason a maximum shell size can be supplied.

The available price function for THex_1_2 are all of those available for the countercurrent model plus

```
Cost = C1 + C2*N*(Area/N)^C3
Cost = C1 + C2*N
Cost = C1 + C2*N + C3*Area^C4
```

TRetro_Hex_Count model:

The Retrofit Counter Current Heat Exchanger model is derived from THex_Count with a few added elements. Calculation of heat exchanger area is identical with its ancestors' method. However, the way the cost is calculated is somewhat different. The retrofit model holds a value for the existing heat exchanger area (AExist).

Further the retrofit model has another property that is not directly visible for the user. That is a retrofit HEN node cannot be removed during the search. The heat load can be set to zero but since removal of an existing exchanger - in general - is associated with an investment the retrofit node should always be kept in the HEN (at least in the internal representation).

The available price functions :

```
Cost = C1 + C2*(Area-AExist)                          if ΔArea > 0
       0                                              if ΔArea <= 0

Cost = C1 + C2*(Area-AExist)^C3                       if ΔArea > 0
       0                                              if ΔArea <= 0

Cost = C1*N_Units + N_shells*C2*(ΔA/N_shells)^C3      if ΔArea > 0
       0                                              if ΔArea <= 0
```

where

```
N_Units = Trunc(ΔA/C4)                          {additional units}
N_shells = 1+Trunc(DeltaArea/C5)                {additional shells}
```

The last one is a pseudo tube and shell price function taken from Shokoya (1992).

In addition to these price functions, a special retrofit price function is derived that explicitly should take into account the cost of removing area from an existing exchanger.

```
Cost = C1 + Area*(C2-C1)/AExist                 if A < (1-C3)*AExist
       C2*Abs(Area-AExist)/(C3*AExist)          if A < (1+C3)*AExist
       C2 + C4*(Area-AExist)^C5                 if A > (1+C3)*AExist
```

where C1 represents the cost of removing the exchanger, C2 the first cost of altering the existing exchanger, C3 is a fraction of the existing exchanger (typically 0.02 - 0.10), C4 is the area price and C5 is the area exponent. An outline of the proposed price function is shown in Figure 6.5.4.

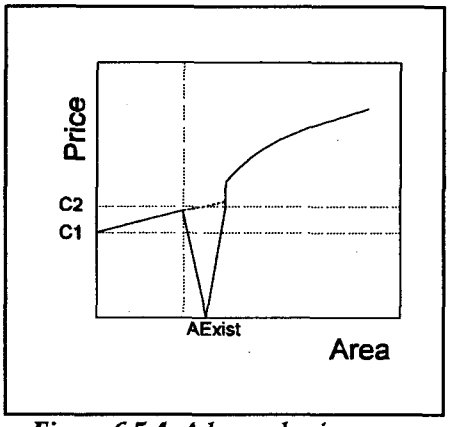


Figure 6.5.4. Advanced price-function for retrofit heat exchangers

TRetro_Hex_1_2 model:

This simple retrofit model is based on the ancestor model - THex_1_2 - with the additional property - Existing Heat Exchanger Area AExist. Calculation of number of shells follows the ancestors' method. The major difference between THex_1_2 and TRetro_Hex_1_2 is the associated price functions.

All price functions for TRetro_Hex_Count can be used plus:

```
Cost =  C1*N_Units + C2*DN_Shells*(DA/N_Shells)^C3   if DArea > 0
        0                                           if DArea <= 0
```

where

```
ΔN_shells = N_shells - Exist_N_shells          {additional shells}
N_Units = Trunc(ΔA/C4)                          {additional units}
```

Splitter and Mixer nodes (TSplitNode and TCombineNode):

Traditionally no cost has been associated with splits and mixers in HEN synthesis. It is, however, often been concluded that the fewer splits the better. Grossmann (1992) thus argues that using no stream split constraints can lead to preferable solutions despite a slight rise in capital costs. It seems a little strange first to define the objective strictly, then using a complex mathematical method to solve the problem and then finally use an undefined personal preference to evaluate the solution. It seems more rigorous to assign a specific cost associated with a stream split. In *HEN Explorer* every split node has its own associated price function.

Currently only one split and one mix node model are implemented. The methods involved in these HEN nodes are quite simple. They just contain methods for calculating mass and energy balances.

Utility nodes:

All utility models are derived from the *TGenirc_Utility* object, which in turn is derived from the *THen_Node*. A distinct limitation in current implementation is that the *Utility Nodes* only can be placed at the end of each stream and that only one utility is available for each stream. For all problems studied in this work this limitation, however, has had very little effect. The utility objects hold methods to calculate the cost (capital and operation) associated with it. The actual heat load is calculated by its parent object (TNodeStream).

In *HEN Explorer* three general utility models are available:

1. TExchanger_Utility
2. TFurnace_Utility
3. TEmpty_Utility

TExchanger_Utility model:

The TExchanger_Utility model is the most often used model. This is the model to use when the utility is served with a utility process stream such as steam, cooling water etc. The TExchanger_Utility thus contains a utility process stream derived from the process stream hierarchy and a heat exchanger derived from the HEN unit hierarchy. Capital cost is calculated by the price functions described for heat exchangers, while energy cost is calculated using another price function. Only a simple price function for energy cost is available

```
Energy Cost = C1 * Heat Load
```

This energy cost function is currently the only one available for all utility models.

TFurnace_Utility model:

The TFurnace_utility model represents a typical fuel fired furnace met in refineries. The capital cost associated with the furnace is calculated as a function of the heat load (Q). Currently three price functions are available:

```
Cost = C1*Q
Cost = C1 + C2*Q
Cost = C1 + C2*Q^C3
```

TEmpty_Utility model:

The TEmpty_Utility is - as the name suggests - a utility that disregards the utility need. This model is used for process streams where there is no final target temperature. A typical example is the flue gas where the resulting temperature depends on the optimal heat recovery rate. The empty utility model simply sets the associated energy and capital costs to zero.

6.6 Simulated Annealing algorithm in HEN Explorer

Most effort has been made in extending the scope for HEN synthesis. There has therefore only been made limited work on improving the optimisation algorithm. Implementation of simulated annealing in HEN Explorer thus closely follows the implementation proposed by Dolan et al. (1990) (described in chapter 5.3). The move set defined by Dolan et al. is:

> *Add exchanger:* A new exchanger (two exchanger nodes) is added randomly in the network. The heat load is chosen as a random fraction of the minimum utility need from the two streams. After the exchanger is inserted the energy and design equations are calculated along with the resulting change in objective (ΔC).
>
> *Delete exchanger:* A random exchanger in the network is selected and deleted. All affected nodes are then recalculated.
>
> *Change q:* A random exchanger is selected and the heat load (q) is changed. The maximum change in q is 20 % of the current heat load.
>
> *Shift q:* Shifting heat load between two exchangers on the same randomly chosen stream. The maximum amount of heat shifted is set to 40 % of the minimum of the two heat loads.
>
> *Add split and exchanger:* Adding a split and combiner with a new exchanger on the split stream.
>
> *Change split ratio:* Changing the split ratio for a random splitnode with a random fraction between -0.2 and 0.2. Split ratios greater than unity or less than zero are set to unity or zero respectively.

One minor difference is, when Dolan et al. give equal probability to every move, HEN Explorer is able to assign individual probability for each move. Further HEN Explorer will impose an upper limit in the number of matches and splits allowed in the network. The latter modification prevents a huge number of heat exchangers in the network during the search. Initial tests showed that the number of exchangers could indeed be very high in the beginning of a search.

Tests have also been made using an initial network. Nielsen et al. (1994) has thus used a three step procedure with Pinch analysis (Superatgergeting), MILP and HEN Explorer. The three step procedure showed that the computational time could be decreased significantly with limited reduction in solution optimality. In many practical cases there is, however, not much emphasise on computational time. This is the primary reason why only limited effort has been invested in increasing the computational performance. The need for improvement will probably occur when expanding the synthesis problem into interfacing process units. This has been beyond the scope of this thesis but few thoughts on improvement have arise during the work.

Adaptive search Tests has disclosed that the type of moves that is most likely to be accepted changes during the search. Initially the probability of accepting moves is equally distributed among the moves. Later during the search configurational changes

become more and more difficult. It might be interesting to allow the probability distribution for attempting a move to change during the search in a way that favour configurational changes in the beginning and then later on favour the continuos changes.

6.7 Improved framework - Summary.

This chapter has described a new framework for heat exchanger network synthesis. The advantage of the new framework is that it supplies the developer with a platform where models can be derived systematically from generalised models. Two conceptual model hierarchies are proposed based on the functional description of process streams and network units. The framework is implemented using object oriented programming.

7
GENERAL GUIDELINES FOR EFFICIENT USE OF ENERGY SYSTEM SYNTHESIS TOOLS

Both mathematical methods and pinch analysis have proved to be very efficient when applied to different energy related synthesis problems. Together with applied heuristics these methods have complementary advantages (Nielsen et al. 1994).The question is, however, how and when to apply the three different approaches. Nielsen et al. 1994 discussed this issue in view of abstraction levels. In chapter 1.3 an abstract model of the synthesis work was outlined in terms of *Process Synthesis Cycle*. In chapter 2.5 the uncertainties were compared with the accuracy of the synthesis methods. In this chapter a general approach will be outlined based on the theoretical and practical work carried out during this research.

A general approach should first of all not constrain the practitioner needless. Further the approach should be straight forward and transparent to the user. One thing that also should be in mind is software availability. Much of the work presented in literature are based on advanced software tools that are not readily available to the industrial user. A general approach applicable for a wide range of end users should thus be based on commercial tools and transparent methods. This excludes a large part of the efficient methods developed within mathematical programming (at least for now).

While waiting for better synthesis software, optimum use of available tools must be secured. The cornerstone in practical synthesis studies (including energy analysis) is the process simulator. A process simulator is ideal for *what if* evaluations. Some simulators even include optimisers that can optimise a given objective function by changing a set of design variables. Further some simulators have a build-in Pinch based targeting tool.

The essential problem with synthesis based on process simulation is handling of the combinatorial aspect. When looking at energy system synthesis heat exchanger network plays an important part. Instead of designing a specific heat exchanger network, the process composite curve can be used. A complex combinatorial problem is thus replaced with a simple targeting problem. Targeting method can thus take much work out of the flowsheeting problem. When different flowsheet alternatives are considered the targeting procedure can estimate the effect. This approach has been used by Lang et al. (1988), who treated the heat integration part as a black box.

The approach proposed here is simple and requires only a process simulator with a build-in pinch targeting tool (for example HYSIM that is used throughout this study). A simple procedure based on this approach is

1. Obtain base case configuration.

2. Remove all utility streams (non kernel process streams) - Conceptual model.
3. Select basic utility concept(s).
4. Set initial/Update kernel process parameters and key utility parameters.
5. Supply all process streams with simple utilities (coolers and heaters).
6. Calculate pinch targets (minimum energy use based on ΔT_{min} or minimum approach temperature in threshold problems).
7. Repeat step 4-6 while optimising energy recovery, material conversion or power production.
8. Design heat exchanger network for optimised process and utility concept.

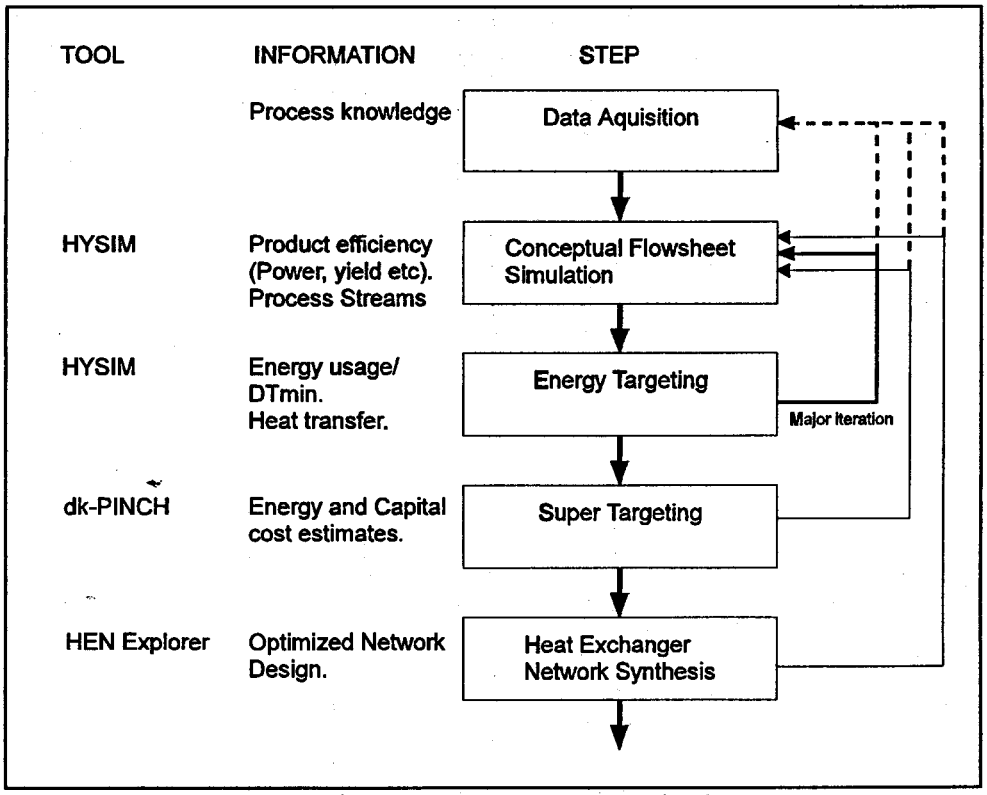


Figure 7.1 General procedure for process energy system synthesis.

This approach can be used as a standard concept. An adapted model based on software available in the current research is outlined in Figure 7.1. With the Synthesis Cycle in mind, first step is to make a preliminary data acquisition, where it is learned how the process operates and what is important for the manufacturer. Using this insight a model without process to process heat exchangers of the flowsheet can be set up in the simulator (HYSIM). This simulation gives the initial process streams and basic plant characteristic (Power production, production yield etc.) with no detail on how to supply the required energy. Then a simple energy targeting is applied, that calculates the minimum energy requirement based on a specified ΔT_{min} or the ΔT_{min} based on a specified energy usage. Simulation and energy targeting can be carried out

within the HYSIM simulation software. Simulation and energy targeting give an overview of the major operational costs (energy, raw material, product costs/sales etc.) and also an overview of the heat transfer process via the process composite curve. This insight can be used in updating the conceptual simulation model (which might require additional data acquisition). The number of iterations depends heavily on the users' process knowledge and ability to interpret the process composite curve in view of the conceptual models optimisation parameters. In other words, how process influence changes in the process composite curves.

So far targeting has been done with no proper energy-capital trade off for the heat exchanger network. Instead several approach temperatures can be imposed such that we obtain two or more conceptually optimised models (e.g. ΔT_{min}=10,20 and 40°C). When leaving the process simulator the optimised conceptual designs can be fed to a stand alone pinch analysis tool (dk-PINCH, Nielsen 1993) with area targeting capabilities. Here an energy-capital trade off (supertargeting) can be made for the conceptual models. The results can be used for selecting between the alternatives or used for updating the conceptual optimisation.

Finally the detailed heat exchanger network is designed. The process stream is fed to the HEN synthesis tool (HEN Explorer) with no imposed minimum approach temperature. For complex problems (non uniform heat transfer coefficients, non counter current heat exchanger, complex price models etc.) the HEN synthesis may disclose trade off's (Unit, area , energy) not found with supertargeting. Therefore it might be necessary to iterate a couple of times through the total synthesis procedure.

This procedure has been applied in modified forms in three synthesis studies. In the first study (Nielsen and Hansen, 1995 and chapter 10) the nitric acid process was evaluated for enhanced energy efficiency. In the second study (chapter 9) a new power cycle is evaluated. Finally in chapter 11 the sulphuric acid process is considered. All studies demonstrate that the above procedure makes it easy to evaluate far more alternatives than with conventional simulation trial and error approaches.

Finally a comment should be added regarding heuristics. Heuristics represent an intuitive approach based on intelligent reasoning based on experience, thermodynamic insight, mathematical knowledge etc. Heuristics are used at every level of method development and application problems. Efficient use of heuristics is probably still the key to successful synthesis. In the nitric acid process evaluation, heuristics based on exergy insight and experience from power production technologies were the key to the successful improvements. The above procedure was merely used for optimisation on a more detailed level. In the power plant analysis heuristics was used to streamline the approach using thermodynamic insight.

Heuristics are thus invaluable in modern process synthesis. Realistic formulations of practical problems are likely to lead to mathematical problems which are difficult or even impossible to solve rigorously. Heuristics are thus an essential element in searching for approximate solutions (decomposition, model simplification etc.).

8
HEAT EXCHANGER NETWORK SYNTHESIS WITH *HEN EXPLORER*

In this chapter the proposed framework for HEN synthesis, implemented in *HEN Explorer*, is tested for a range of different problems. First it is tested with standard problems met in literature to evaluate its efficiency. This includes conventional problems with constant heat capacity and countercurrent heat transfer. Subsequently more realistic problem formulations include some of the advanced elements of HEN Explorer. All the problems and results are documented in appendix 7.

8.1 Simple design problems.

Ahmad (1985) discusses the importance of correct initialisation of HENs. He introduces the driving force plot and the remaining problem analysis to optimise HEN for a given energy target. The problems used by Ahmad are simple and well documented.

In table 8.1.1 the data for Ahmads problem P1 is given

Table 8.1.1 Streams	TS (°C)	TT (°C)	CP (kW/K)	h (kW/m²K)
H1	300	80	0.3	0.4
H2	200	40	0.45	0.4
C1	40	180	0.4	0.4
C2	140	280	0.6	0.4
Heat exchanger capital cost equation:		300 $A^{0.5}$	($/yr)	
Hot utility (400-399°C) costs:		110	($/(kW.yr)	
Cold utility (10-11°C) costs:		12.2	($/(kW.yr)	
Utility heat transfer coeff.		0.4	(kW/m²K)	

Ahmad uses supertargeting to find the optimal heat recovery approach temperature ΔT_{min}. He then uses the pinch design method to establish four different designs. He finally relaxes the energy target using loops and paths to trade off energy for capital.

HEN Explorer is applied to this problem with no assumption of ΔT_{min}. Nine different initial seeds are used. In table 8.1.2 the solutions proposed by Ahmad (1985) are listed together with selected results obtained with *HEN Explorer*.

Table 8.1.2 Case	Energy use (kW)	Area (m^2)	Units Process/ utility	Total cost ($/yr)
Supertarget	32.5	26.8		8056
Ahmad P1A	32.3	29.2		7875
Ahmad P1B	32.4	28.5		7917
Ahmad P1C	36.8	24.1		7775
Ahmad P1D	36.9	23.4		7834
HEN Explorer A01	33.1	32.3	3 / 3	7419
HEN Explorer A02	37.0	23.8	2 / 3	7405
HEN Explorer A09	33.5	31.9	3 / 3	7410

From table 8.1.2 a considerable improvement is noticed (5%), using HEN Explorer compared with the solutions proposed by Ahmad. This improvement is mainly due to the low area exponent (0.5), which favours few but large exchangers. There is thus a considerable trade off between number of units and heat exchanger area, that makes it profitable to transfer heat across the pinch. The advantage with HEN Explorer is that it is able to exploit these hidden trade offs.

Similarly HEN Explorer is applied to two other simple cases supplied by Ahmad (1985). His results together with results obtained with HEN Explorer are shown in Table 8.1.3.

Table 8.1.3		Energy use kW	Area m^2	Units Process/utility	Total cost $/yr
P2	Supertargeting	12	75	7	8650
	Ahmad	11.7	68.0	not given	6889
	HEN Explorer	11.8	88.7	4/3	6850
P3	Supertargeting	111.0	86.6	7	20218
	Ahmad	112.2	93.5	not given	19668
	HEN Explorer	107	101.9	3/4	19230

The last of the simple problems given by Ahmad is a larger problem with six hot streams and 4 cold streams. In this case the cost equation is given by: Cost = 60 Area ($/yr). There is thus no incentive to minimise the number of units in the network. This is reflected in the solutions obtained with HEN Explorer for the original formulation. These solutions all had a high number of units (25-30 units). To decrease the resulting number of units an additional cost (50000 $/unit) was associated to each exchanger,

representing first cost. This resulted much simpler but slightly more expensive network (Table 8.1.4).

Table 8.1.4 Ahmad case study	Energy use kW	Area m^2	Units Process/Utility	Total Cost M$/yr
Ahmad	22356.5	57551	8/7	5.94
HEN Explorer original formulation	20752	57071	20/6	5.73
HEN Explorer First cost included	21290	57112	6/8	5.79

This problem also outlines one of the problems that can occur when using HEN Explorer on ill defined problem. Since HEN Explorer is solely driven by the objective function this has to include all essential cost items. Where Pinch Design Method is based on sequential approach where the number of units can be controlled by the designer, HEN Explorer requires, that it is possible to find the optimal number of units based on cost equations. Thus there should always be a first cost or an area exponent in the heat exchanger cost equation. It should be noted that this requirement is also in line with the real world problems.

These simple problems document that *HEN Explorer* indeed is competitive with other approaches for simple problems.

8.2 Heat exchanger network with non-uniform heat transfer coefficients.

In the previous section the heat transfer coefficients where uniform. Earlier it has been shown that non-uniform heat transfer coefficients have an effect on the overall heat exchanger network targeting (Chapter 3.7). In this section example problems with non uniform heat transfer coefficients are evaluated.

The first example has been used by Floudas et al. (1986) and by Dolan et al. (1989,90). It is a seven stream problem. Data for the problem is given in table 8.2.1.

Table 8.2.1 Floudas et al 1986	TS K	TT K	CP kW/K	h kW/m^2K
C1	288.8	650.0	24.795	0.8753
H1	630.6	338.9	7.913	1.6097
H2	583.3	505.6	5.803	0.7265
H3	555.6	319.4	2.374	0.5586
H4	494.4	447.2	31.652	0.7299

H5	477.8	311.1	6.331	0.3541
H6	422.2	383.3	65.943	0.4848
CW	300	333.3	-	0.6324

Heat exchanger capital cost equation:	1300 $A^{0.6}$	($/yr)
Furnace capital cost equation	321.089 $Q^{0.7}$	($/yr)
Hot utility costs:	174.022	($/(kW.yr)
Cold utility costs:	4.634	($/(kW.yr)

Floudas et al. (1986) found with their approach an optimum solution with a cost of $645,600: Dolan et al. (1990) later found a new optimum - $640,200.

With *HEN Explorer* it has not been possible to obtain better solution than that of Dolan et al. (1990). The best solution found with *HEN Explorer* is $641,618. This solution is, however, so close to the best known solution that it can be concluded, that *HEN Explorer* also produces network close to the optimum for problems with varying heat transfer coefficients.

There has so far been no focus on computer time consumption. The above example problem is also used to evaluate the choice between multiple fast annealings and few slow annealings. With constant CPU time a number of optimisations are carried out.

Table 8.2.2 Number of runs	Best solution	Average
1 (slow annealing)	646,796	646,796
2	646,356	652,929
3	648,203	664,271
7 (fast annealing)	651,500	683,670

The results indicate that in this case using few slow annealing schedules is better than to carry out many fast annealings. To validate this result, two further tests were made.

Table 8.2.3 Number of runs	Best of best solutions	worst of best solutions	Average optimum solution
1	646,382	652,153	648,444
2	646,356	661,426	651,996
3	648,203	651,220	649,943
7	648,208	651,500	649,404

Table 8.2.3 indicates that finding near optimum solution requires slow scheduling. It does, however, also indicate that using few slow schedules can result in an inferior solution (see "worst of best solution" column). The expected behaviour can be read of the average column. Here the average of the best solutions is given. The results show that all approaches are expected to give equally good results.

Based on these results, supplemented with the general experience in using *HEN Explorer*, it is recommended to use at least 3 runs with different initial seeds.

The trade off between computational effort and quality of the result is, however, no real issue in most practical studies. In most cases the computational time is of no importance as long it is restricted to be within hours or days. This seems to be the case with the problems tested in the present work

8.3 Optimisation with tube and shell heat exchanger models.

All of the previous examples have featured constant heat capacity and only countercurrent heat exchangers are used. This section treats the more detailed problem formulations where tube and shell exchangers are assumed. The first three problems listed in table 8.3.1 are identical to examples P1 - P3 used in section 8.1, except that this time a tube and shell model is used. The last example is taken from Ahmad *et al.* (1990). The heat exchanger design follows that described by Ahmad (1985) with a specified $X_p = 0.9$. Ten runs are made for each problem.

Table 8.3.1		Energy use kW	Area m^2	Units Process + utility	Shells	Total cost \$/yr
P1	Supertargeting	43.8	18.26	n.a	9	9168
	Ahmad	40.0	21.38	5+2	11	9426
	HEN Explore	45.3	16.21	4+3	9	9204
P2	Supertargeting	41.0	44.32	n.a.	14	12605
	Ahmad	50.0	42.08	5+2	13	12870
	HEN Explorer	34.15	55.83	6+3	15	12306
P3	Supertargeting	125.4	67.47	n.a.	7	21112
	Ahmad	138.0				
	HEN Explorer	115.7	66.45	3+4	9	19630
P4	Supertageting	10125	n.a.	n.a.	n.a.	n.a
	Ahmad *et al.*	10125	5862	11+4	19	$1.663\ 10^6$
	HEN Explorer	9659	6937	10+5	19	$1.541\ 10^6$

Table 8.3.1 clearly shows that *HEN Explorer* is able to find the better solutions for HEN synthesis with more detailed modelling.

8.4 Retrofitting Heat Exchanger Network with Explorer.

The retrofitting capability of Explorer is illustrated with two examples from Shokoya (1992).

Example 1

The first example is a five stream problem with an existing network (Topmost network in Figure 8.4.1). The task given in the original presentation is to find the best retrofitted network (total costs) that fits a pay back limit of two years.

Streams	TS (°C)	TT (°C)	CP (kW/K)	h (kW/m²K)
H1	165.0	95.0	148.0	0.45
H2	240.0	65.0	86.4	0.55
C1	125.0	220.0	139.0	0.35
C2	61.0	192.0	54.6	0.40
C3	70.0	185.0	62.0	0.64

Heat Exchanger Capital Cost equation: $8600 + 835\ A^{0.83}$ ($)
Hot utility cost: 60.00 ($/kW.yr)
Cold utility cost: 0.0 ($/kW.yr)

A is the area of the heat exchanger in m²

Table 8.4.1 Stream and cost data for example 1 (Shokoya 1992).

With the current version of Explorer the objective function is based on the total cost based on a time serie (for example. Net Present Value). Therefore to analyse the retrofit problem there will be assumed a time period under which the results will be determined.

Table 8.4.2 Exchanger Number	Existing Area (m²)
1	132.6
2	467.2
3	898.2
4	742.1

Shokoya (1992) uses countercurrent heat exchanger models for area calculation, which for comparison will be adopted. The best network obtained by using the area matrix based method features one split, two new exchangers and modification of one existing exchanger. The retrofit network has an energy reduction of 1860 kW (60 %) with 600 m^2 in additional heat exchange area. This results in a pay back of 2 years.

When applying Explorer to the problem, several parameters must be set. Since the problem is small a relative fast cooling schedule can be expected (parameter d in the range 0.1 - 2, Markov Length 100 - 400). The initial annealing temperature is initially set to 900000 but later reduced to 100000. The results from Explorer are outlined in table 8.4.3. The layout of the different alternatives are shown in Figure 8.4.1.

Table 8.4.3 Case	Energy reduction kW	Exchanger costs $	Energy savings $/yr	Pay Back yr
Shokoya	1860	223200	111600	2
1	2133	246353	127923	1.93
2	2246	240225	134735	1.78
3	2184	242159	131029	1.85

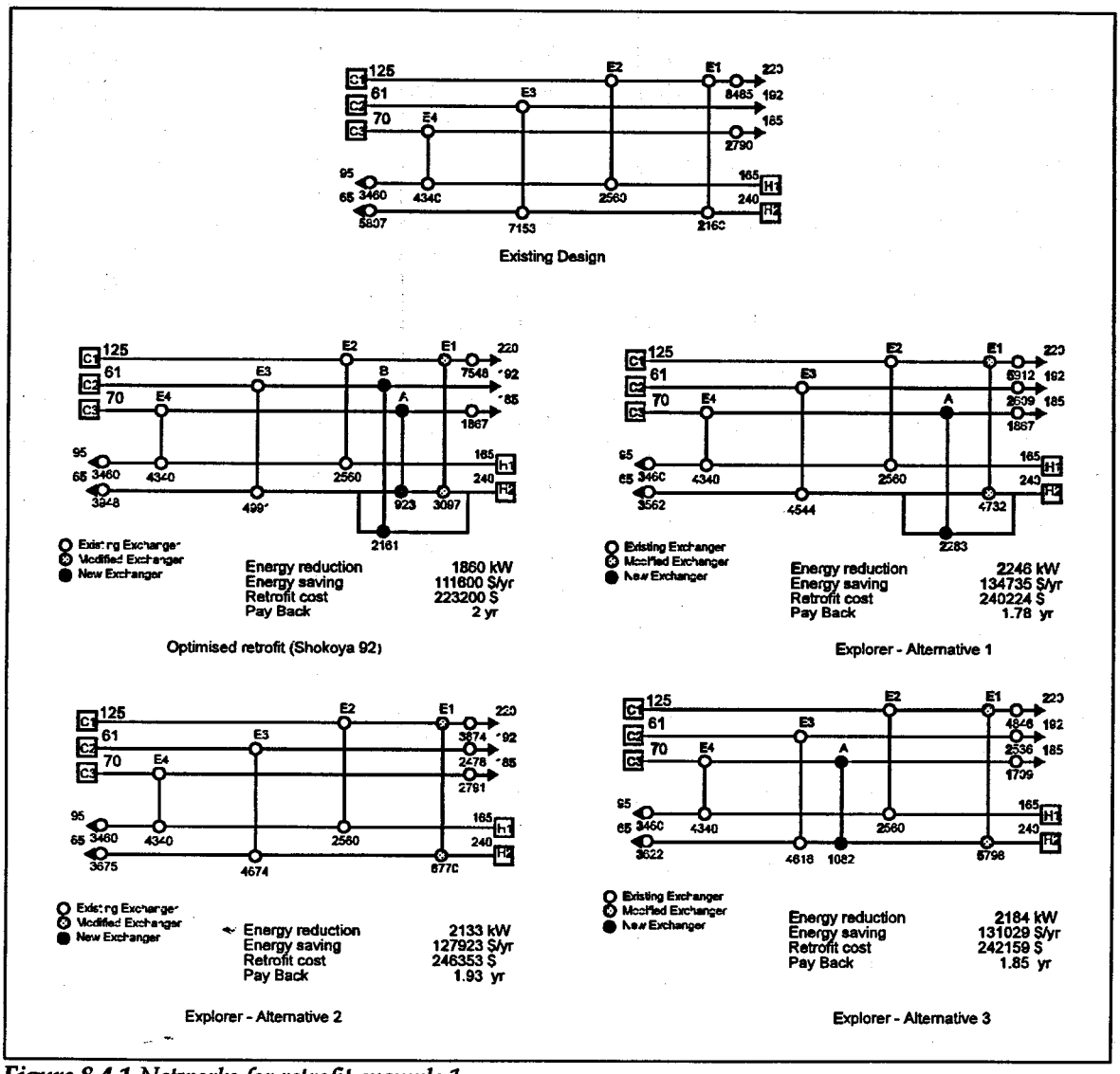


Figure 8.4.1 Networks for retrofit example 1.

Example 2

Example 2 represents debottlenecking of a crude unit, where the task is to design the heat exchanger network for a 10 % increase in flowrate. A simplified flowsheet of the crude unit is given in Figure 3 (Shokoya 1992). The bottleneck of plant is the furnace capacity. Presently the furnace can yield 95 MW, which is not sufficient when the flowrates are increased. Stream data and exchanger sizes for the original flows are given in table 8.4.4.

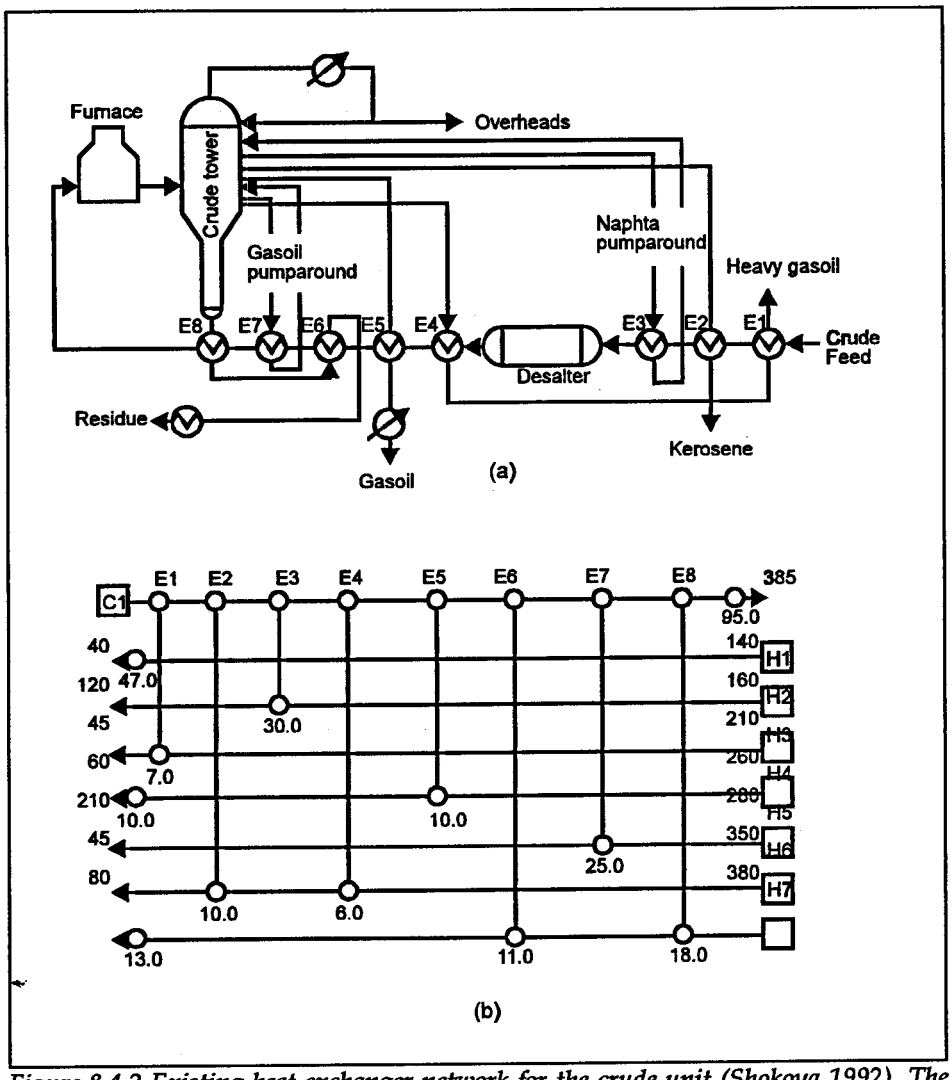


Figure 8.4.2 Existing heat exchanger network for the crude unit (Shokoya 1992). The heat exchanger network is extracted from the complete flowsheet (a) and represented in a grid diagram.

Table 8.4.4 Streams	TS (°C)	TT (°C)	CP (kW/K)	h (kW/m²K)
C1	10 130 270	130 270 385	391.670 (430.837) 500.000 (550.000) 826.090 (908.699)	0.50 0.70 0.90
H1	140	40	470.000 (517.000)	0.20
H2	160	120	750.000 (825.000)	1.50
H3	210	45	42.420 (46.662)	0.80
H4	260	60	100.000 (110.000)	0.70
H5	280	210	357.140 (392.854)	1.0
H6	350	170	55.560 (61.116)	0.50

	170	45	48.000 (52.800)	0.40
H7	380 160	160 80	145.460 (160.006) 125.000 (137.500)	0.40 0.30
Existing exchangers				
E1	255.0		E5	605.0
E2	595.0		E6	1288.0
E3	1744		E7	1733.0
E4	133		E8	1092.0

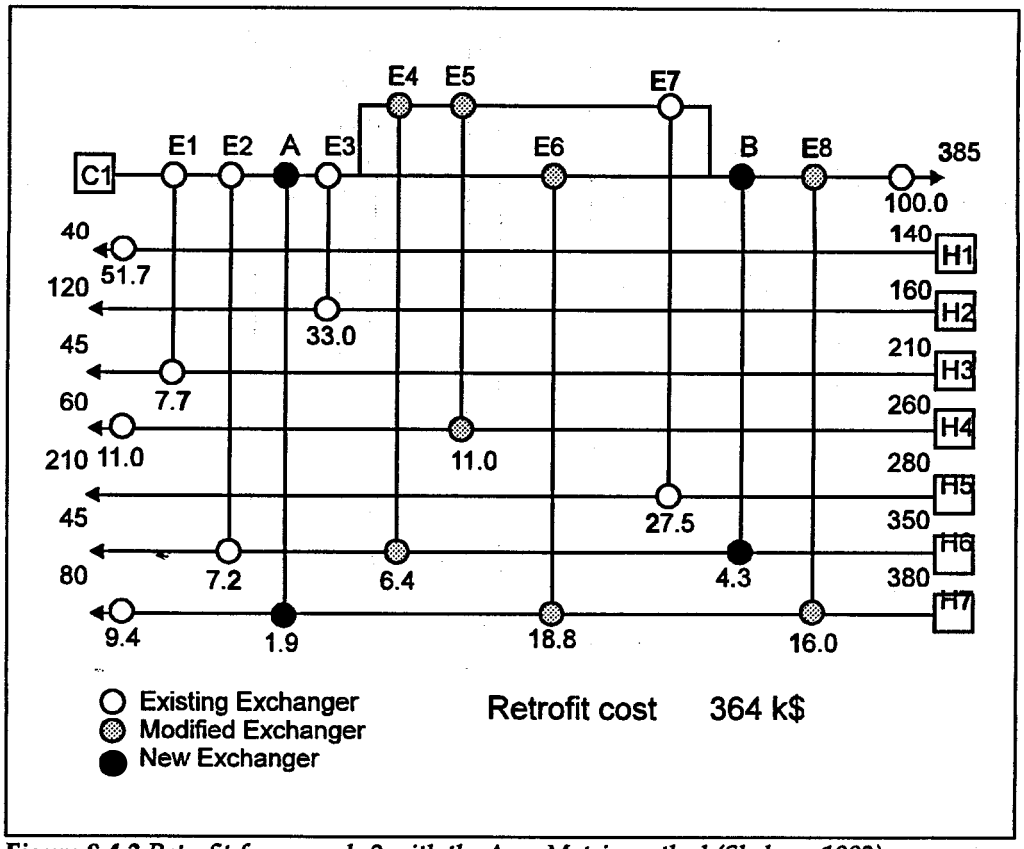


Figure 8.4.3 Retrofit for example 2 with the Area Matrix method (Shokoya 1992).

Shokya uses the Area Matrix method to retrofit the network. Her results are outlined in Figure 8.4. *HEN Explorer* is applied to the same problem. In table 8.4.5 the results from *HEN Explorer* are compared with those obtained with the Area Matrix method.

Table 8.4.5 Result	New units	New Area m²	Retrofit units	Retrofit area m²	Total cost K$
Shokoya	2	321	4	980	364.0
HEN Explorer	2	687	3	532	342.3
"	3	2077	2	442	315.0
"	2	766	3	464	324.7
"	2	546	4	754	362.0
"	3	1139	2	124	371.5

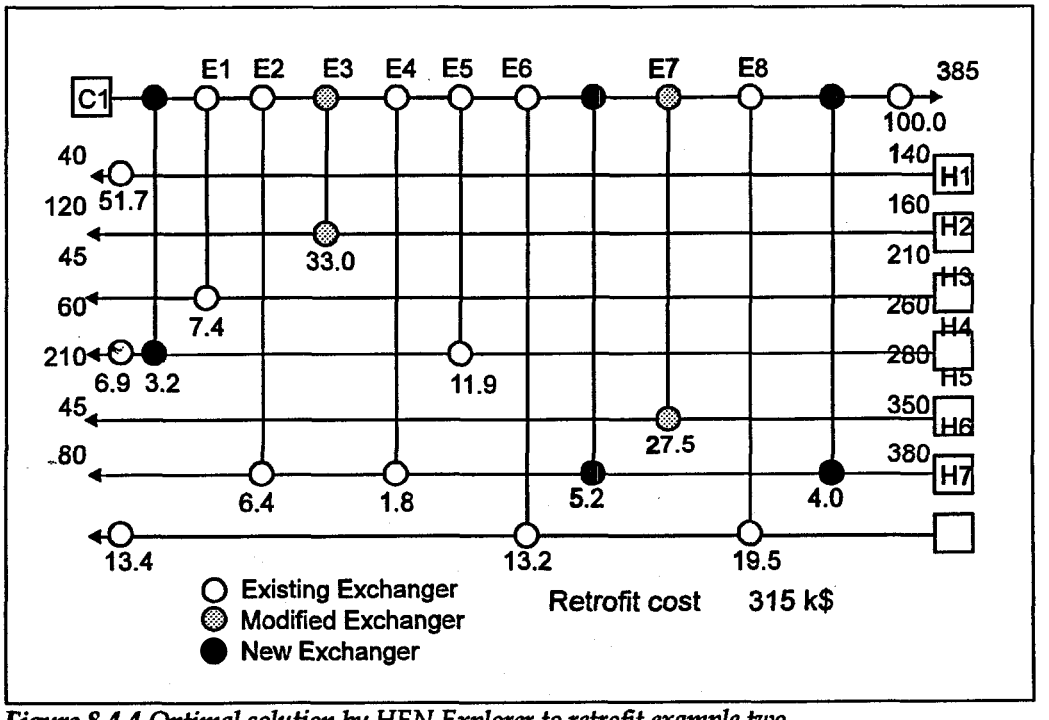


Figure 8.4.4 Optimal solution by HEN Explorer to retrofit example two.

The best network obtained with HEN Explorer is outlined in Figure 8.4.4. A considerable improvement with HEN Explorer is noticed. The modification cost is reduced with 13 % compared with Shokoyas solution. In contrast to the Area Matrix method HEN Explorer exploits the complex trade off between number of units and distribution of area. It can thus be noted that the optimum solution does not feature minimum additional heat exchange area. Compared with Shokoyas solution, the optimum solution found with HEN Explorer requires almost twice as much area. The area is, however, distributed in a way that minimise the associated cost. This example illustrates clearly, that HEN Explorer is able to handle complex trade offs.

8.5 HEN synthesis with HEN Explorer - Summary

HEN Explorer has been tested with a set of literature problems of varying complexity. In all cases HEN Explorer has proven to be efficient. It has the ability to handle complex trade offs simultaneously. This performance is especially of importance when applying complex nonconvex pricefunctions or using enhanced heat exchanger models.

9
SYSTEMATIC OPTIMISATION OF THE HUMID AIR TURBINE CYCLE

The example in this chapter illustrates how the general approach for energy synthesis can be used for power plant optimisation. The framework is the Humid Air Turbine (HAT) cycle (Rao, 1989) which will be introduced. The approach has been tailored to the problem trying to make full use of all available insight and heuristics.

9.1 Introduction to the HAT cycle.

The Humid Air Turbine (HAT) cycle was patented by Flour Daniel (Rao 1989). The cycle uses a working medium of humidified air. The cycle, which in its general form is quite simple compared with other innovative power cycles (e.g. Kalina et al. 1991), is based on recent advances in gas turbine technology. With no top or bottoming cycles the HAT cycle is reported to give efficiencies of over 60% (LHV). The new cycle has been given a considerable interest over the last couple of years. Several studies have aimed at optimising the cycle performance using different process layouts (Xiao et al. 1994, Stecco et al. 1993a,1993b). These studies have been based on a fixed or semi-fixed conceptual layout followed by a parametric optimisation. The aim of this work is to show how a general top down analysis can be applied to the cycle with a considerable gain in the optimisation work. With simple rules based on second law insight and pinch technology an optimisation study can be carried out using a standard process simulator within a few days.

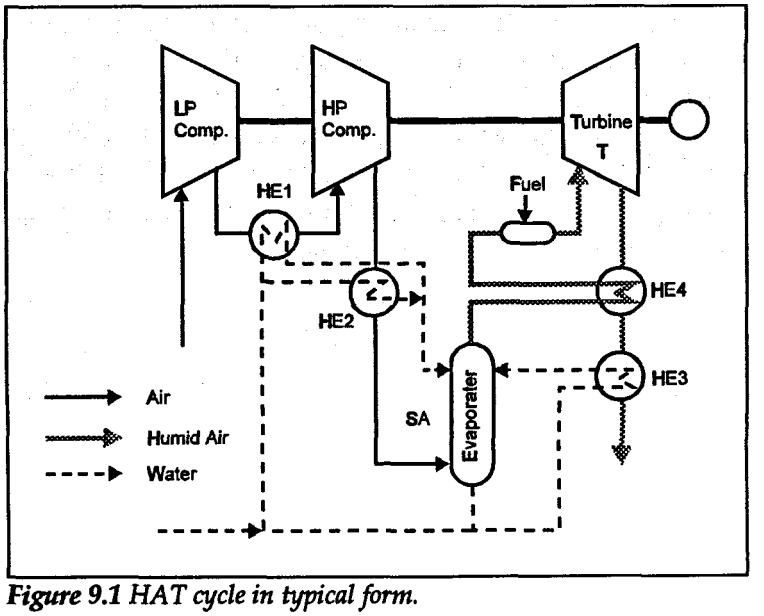


Figure 9.1 HAT cycle in typical form.

The typical layout for the HAT cycle is shown in Figure 9.1. The air is compressed in two stages with an intercooler (HE1). The intercooler gives a lower temperature into the second stage compressor and thus a smaller power consumption. The removed heat is used to heat up some water for the evaporator. After the second compression stage the gas is cooled once more (HE2) before it enters the evaporator (SA). Here the gas meets the hot water in countercurrent flow. This unit gives a simultaneous mass and heat transfer where the water is evaporated at variable temperature. The humidified air is then heated in a regenerator (HE4), where heat from the turbine exit is used to heat the humidified air. In the combuster fuel is injected and burned. The hot gas now enters the gas turbine (T). The tail gas is cooled in two steps. First in the regenerator and after that in a water heater (HE3).

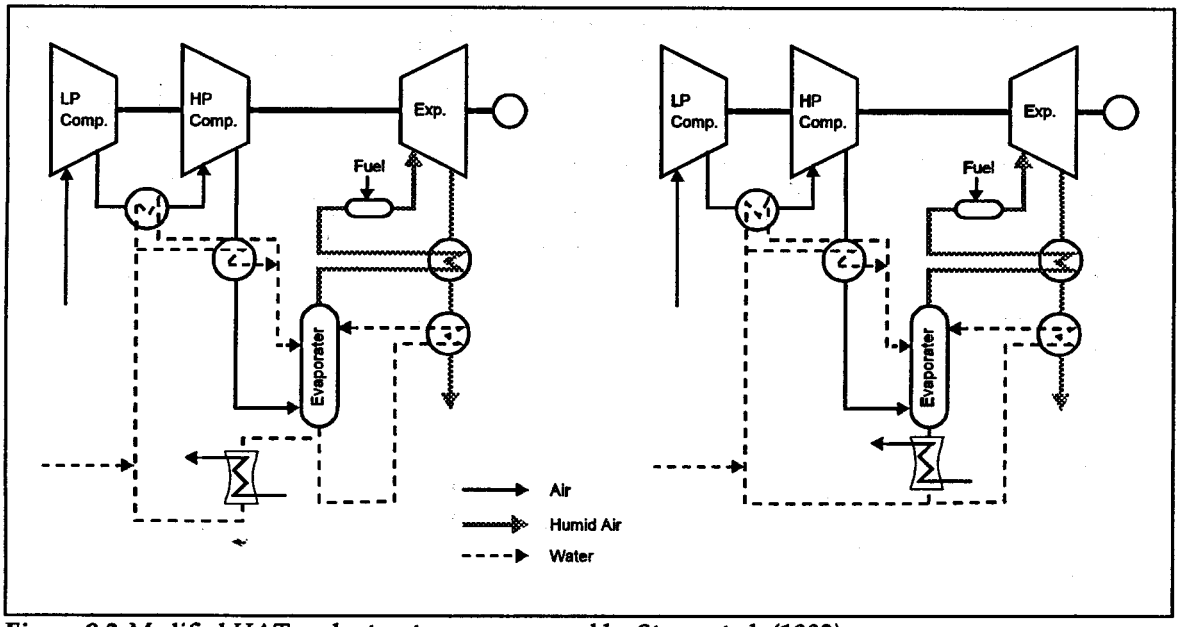


Figure 9.2 Modified HAT cycle structures as proposed by Stecco et al. (1993).

Stecco et al. (1993a,b) propose two variations where a cooling tower is applied to decrease the temperature inlet to second compression stage (Figure 9.2). Xiao et al. (1994) propose an alternative layout based on a superstructure that embed several different heat exchanger configurations (Figure 9.3). Stecco et al. get their results by varying the key parameters for each configuration. In this case they varied the compression ratios for both compressors and the relative humidity at the evaporator outlet. Xiao et al. (1994) optimised the system with an algorithmic approach applying an infeasible path method with a process simulator.

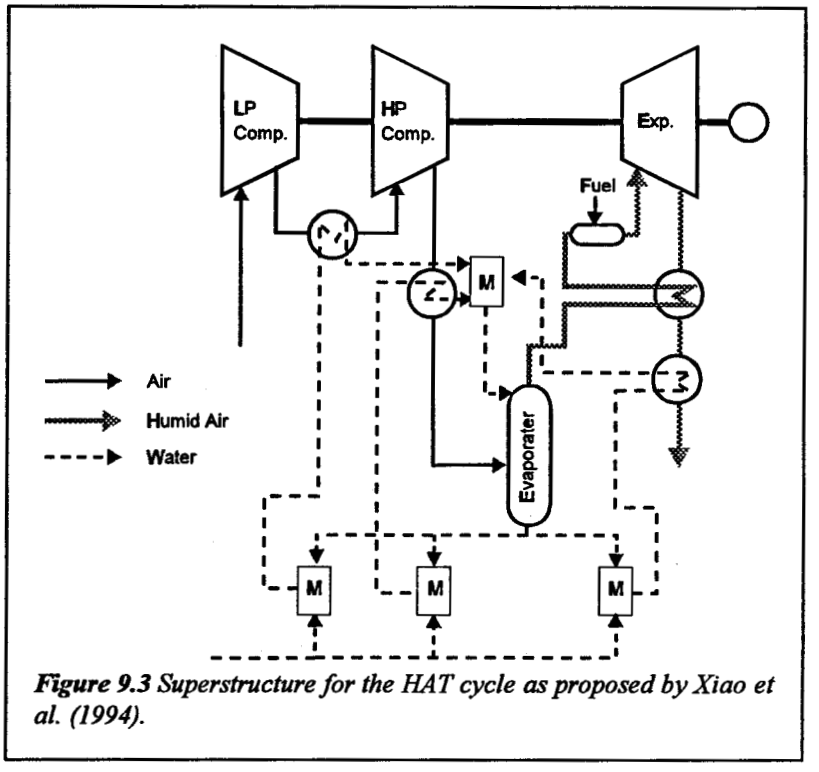


Figure 9.3 Superstructure for the HAT cycle as proposed by Xiao et al. (1994).

9.2 Optimisation of the HAT cycle.

In this case study the simple global approach as outlined in Chapter 7.

1. Obtain base case configuration.
2. Remove all utility streams (non kernel process streams).
3. Select basic utility concept(s).
4. Set initial/Update kernel process parameters and key utility parameters.
5. Serve all process streams with simple utilities.
6. Calculate pinch targets (minimum approach temperature).
7. Repeat step 4-6 while optimising energy recovery, material conversion or power production.
8. Design heat exchanger network for optimised process and utility concept.

The main feature is the two stage design of the heat exchanger network. Individual heat exchangers are removed and replaced with utility exchangers. After that a pinch analysis calculates energy targets (or temperature approach targets for exothermal processes). At that stage the actual heat exchanger network design is not fixed, but the result shows the feasibility of the proposed process design. Now key process parameters can be varied in the search for optimum performance. For each conceptual process design a pinch analysis can show whether a feasible heat exchanger network exists (whether minimum approach temperature is over or below 0). The major

benefit by this general approach is the limited work on heat exchanger network synthesis. In this case the actual network design is carried out as the last step when most other parameters are fixed. One major advantage is that the same conceptual model can be used throughout the analysis.

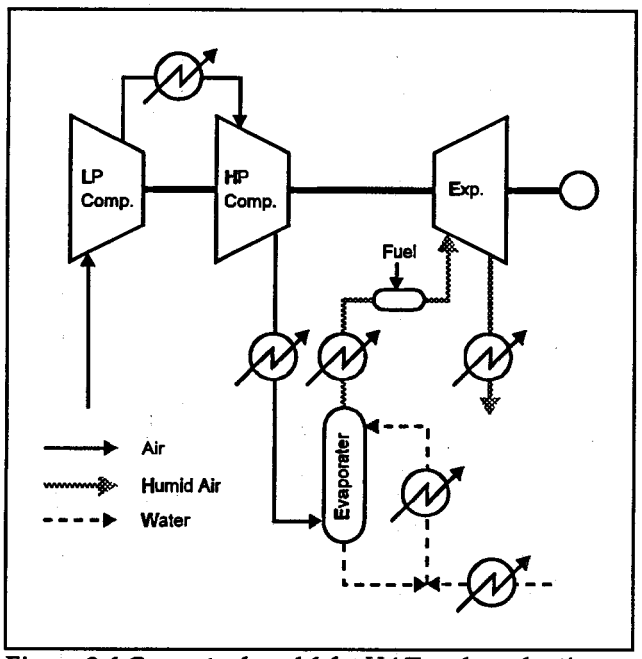


Figure 9.4 Conceptual model for HAT cycle evaluation.

For the HAT cycle a modified approach is suggested based on the particularity of this cycle. If the objective is to maximise the thermal efficiency, some basic exergy consideration can be utilised. The following operations in the HAT power cycle cause exergy losses:

1. Mixing fluids with different temperatures.
2. Heat transfer with temperature driving forces.
3. Irreversibility in the humidifier.
4. Combustion irreversibility.

In this example the irreversibility in the combustion, which can be improved by recycling off-gases (Harvey et al. 1992), will not be considered. Without any quantification it is postulated that optimum performance is obtained when all fluid mixing is done isothermally, heat transfer is carried out with a constant minimum approach temperature and irreversibility in the humidifier is minimised. The irreversibility in the humidifier is caused by a combination of fluid mixing and heat transfer with excessive temperature difference.

A conceptual flowsheet for the HAT cycle is shown in figure 9.4. In this flowsheet no restriction is imposed on placement of individual heat exchangers. It is assumed that all process streams are served by the best available heat source. In the flowsheet this assumption is represented by an external utility. With a given set of process parameters (pressure ratios, humidifier parameters) a targeting analysis can predict the feasibility of the process. With pinch technology the composite curves can be used

to identify thermal inefficiencies (excessive temperature differences). The information can then be used to update the process parameters.

In a typical HAT cycle study (Stecco et al. 1993a,b and Xiao et al. 1994) a set of assumptions is chosen. In this study the assumptions from Stecco et al. are adopted and listed below.

Standard ambient conditions, i.e. temperature 288 K, 1.013 bar	
Maximum turbine inlet temperature	1273 K
Adiabatic compression efficiency	0.85
Adiabatic expansion efficiency	0.90
Combustion chamber efficiency	0.97
Mechanical efficiency	0.98
Electrical efficiency	0.99
Minimum approach temperature, exchangers	10 K
Temperature difference at evaporator exit	2 K
Pressure loss from compression to expansion	3%
Fuel CH_4 with net heat value of	49.99 MJ/kg

In should be noted that Stecco et al. (1993) uses a net heat value of 43.12 MJ/kg for methane. To obtain maximum efficiency the following parameters are optimised

Pressure ratios stage 1 and 2

Evaporator condition (water flow and temperature)

Evolving air flow (kg air/kg fuel)

Simple second law thermodynamic implies that the recuperated temperature should be as close as possible to the turbine exit temperature (i.e. equal to minimum approach temperature). Further we want to keep the composite curves as close as possible over the whole temperature range. Based on this simple insight we are ready to tailoring the approach for HAT cycle optimisation. The optimisation is based on a fixed fuel flow.

1. Set initial/update pressure ratios.
2. Set initial/update evaporator conditions.
3. Set initial/update Air flow.
4. Set initial/update recuperator temperature.
5. Calculate combustion temperature.
6. Repeat 4 and 5 until combustion temperature constraint is reached.
7. Repeat 3-6 until $T_{rec} = T_{exit} - \Delta T_{min}$.
8. Perform ΔT_{min} targeting.
9. Use composite curves to close the gaps between the hot and cold composite curves. This is done by updating evaporator conditions. Repeat step 2 - 9 until the curves are as parallel as possible.
10. Repeat step 1 - 9 over a reasonable pressure range.
11. Design heat exchanger network for selected design parameters.

Although the procedure is quite iterative part of it can be done automatically using a standard process simulator. This is the case for step 3 to 6. Updating of the evaporator condition is a mixture of flow and temperature changes. The choice is dependent of the form of the composite curves. The effect of changing the temperature and massflow rate respectively is illustrated on figure 9.5.

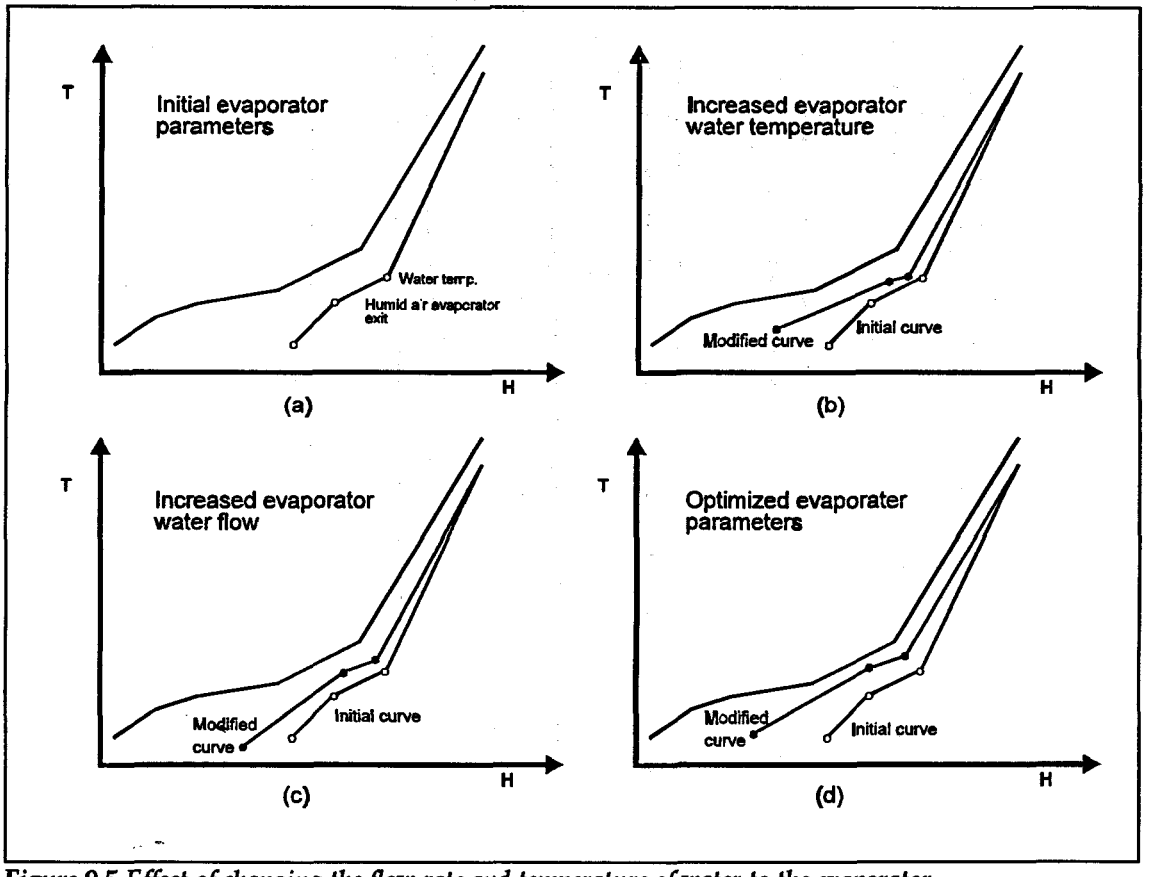


Figure 9.5 Effect of changing the flow rate and temperature of water to the evaporator.

For each set of pressure ratios the only two variables that have to be considered are the water flow rate and temperature. The design problem has thus been reduced significantly. The problem dimension can be reduced even further by using a targeting model for the saturator. Instead of simulating the heat and mass transfer in the saturator an alternative model is used. Water is mixed directly with the combustion air giving a two phase flow. When the mixture is heated, then the water will gradually be evaporated according to its partial pressure. The added water represents the amount of water that is transferred in the saturator. This simplifying model is discussed further in Chapter 10.3, where it is also demonstrated how to retrieve the saturator design from the simple targeting model. The design work is now reduced to select pressure ratios. When the pressure ratios are selected, the amount of water is found by iteration. With a given amount of water, a pinch analysis will give the minimum approach temperature. It typically requires about 4-5 iterations to find the correct flow rate for each set of pressure ratios.

The last help in the design comes when finding the relation between pressure ratios. If the inlet temperatures are identical then the optimal configuration will be when the two ratios are equal. In this case the air inlet of the first compressor will always be slightly colder than the air inlet to the second compressor. Therefore it can be expected that the optimum pressure ratios will be feature a pressure ratio for compressor one that is higher than for compressor two. With this insight the number of iterations can be reduced. The proposed methodology is used for finding the process operation that gives maximum efficiency. The results are given in Table 9.1.

Discharge pressure compressor 1	Discharge pressure compressor 2	ΔT_{min}	Thermal efficiency
3.2	9	10	57.2
2.6	6	10	58.7
2.1	4	10	59.9
2.0	3	10	60.7
1.7	2.5	10	60.6

***Table 9.1** Result of targeting analysis.*

9.3 Discussion HAT power cycle.

This chapter has described how the general approach given in Chapter 7 can be tailored to a specific problem using second law insights and heuristics. The results obtained are in line with those reported by others who used detailed parametric optimisation.

It should be mentioned that the process found with optimum energy efficiency has a major practical drawback. That is it requires a very large airflow rate per produced unit of power. This high airflow rate will result in an economical inferior solution. This aspect is, however, beyond the purpose to pursue any further here.

10
ENERGY SYNTHESIS OF THE NITRIC ACID PROCESS

This chapter shows how the general approach described in Chapter 7 can be tailored for specific optimisation of the nitric acid process. A literature case study has been selected for comparison. The case study was originally presented by Linnhoff during a conference in 1987 (Gaggioli et al. 1991). It was the purpose that the case should be used in a challenge between the school of Exergy Analysis represented by Gaggioli et al. (1991) and the school of Pinch Analysis (Linnhoff and Alanis, 1991).

A new route to improve the energy efficiency of the nitric acid plant is proposed. This new process is optimised and compared with the conventional process.

Finally it is investigated how the process can be implemented in Kemiras HNO_3 unit IV.

10.1 Commercial nitric acid production

Nitric acid plants have attracted much attention because of their low second law efficiencies. The interest has further been enhanced by the competition between two different approaches. The *Pinch Analysis* proposed by Linnhoff and Alanis (1991) and *Exergy Analysis* by Gaggioli et al. (1991). In their respective studies the objective was to integrate a new plant with an on site steam power plant. In this chapter it is only the nitric acid plant that is examined. Most contractors offer plants that are either steam exporting or power exporting (or both). In this chapter the objective is to maximise the net power output with no steam export or import.

The nitric acid process is described in appendix A2, where data for Kemiras unit I to IV are given. The commercial manufacture of HNO_3 of concentration up to 67% involves the following three main reactions:

$$4\ NH_3 + 5\ O_2 = 4\ NO + 6\ H_2O$$
$$2\ NO + O_2 = 2\ NO_2$$
$$3\ NO_2 + H_2O = 2\ HNO_3 + NO$$

The NO in the product stream is stripped off and recycled. This give a net reaction of

$$NH_3 + 2\ O_2 = HNO_3 + H_2O$$

A considerable amount of heat is released (420.45 KJ/mole) by the above reaction. Part of this heat is converted into mechanical work to drive compressors in the process. The base case used by Linnhoff and Alanis (power output mode) was a 890

tpd (100% HNO_3) unit with a net power export of 3965 kW (Figure 10.1). This case gives a specific production of 106 kWh/ton(100% HNO_3). It is, however, a base case that is *not* state of the art. This is reflected by the fact that Kemira's HNO_3 unit IV (UHDE design licensed 1979) has a specific output of ca. 132 kWh/ton(100% HNO_3).

10.2 Case study conventional process (Linnhoff and Alanis 1991, Gaggioli et al. 1991).

This case was originally presented by Linnhoff during a conference in 1987 (Gaggioli et al. 1991). It was the purpose that the case should be used in a challenge between the school of Exergy Analysis represented by Gaggioli et al. (1991) and the school of Pinch Analysis (Linnhoff and Alanis, 1991). The dual pressure nitric acid plant is shown in Figure 10.1 with the detail of flows, compositions, and thermodynamic properties associated with each stream in Table 10.1. Further the compressor and turbine efficiencies are given in Table 10.2. These values are calculated from the stream properties in Table 10.1. Finally a set of constraints are assumed. In this case study it is assumed that the reaction conditions should be considered fixed. This means that the converter temperature should be kept at 840 °C and the pressure at 3.3 bar. The oxidisation heat is assumed released linearly in the temperature interval imposed by Table 10.1. Finally the tail gas inlet temperature to the expander is limited to 700 C. Some of these constraints can be discussed, but so far they can be viewed as safe side constraints and will be used in this case study.

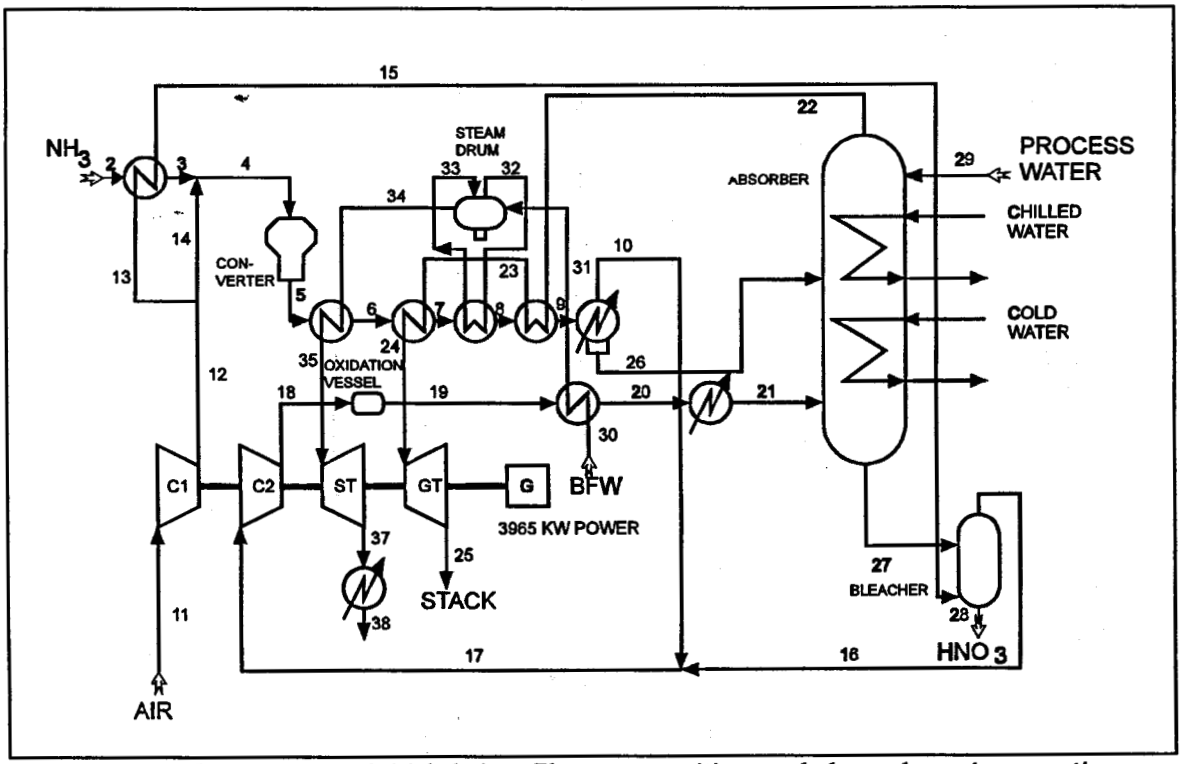


Figure 10.1. HNO_3 process initial design. Flows, compositions and thermodynamic properties are given in Table 10.1, isentropic efficiencies for turbines and compressors in Table 10.2.

There are several different paths for improving the net power output from the process plant. In the studies of the above mentioned authors basically two parameters are examined

a) Increased gas turbine temperature.

b) Increased steam production.

The optimum is then found as a combination of the two parameters.

Associated with option b) minor changes in pressure have been included. Optimisation of the power production with these options can be done in two steps using the principle of pinch analysis: 1) Targeting 2) Design

Flow	T	P	Flow						H(T,P)
	°C	Bar	Kg/hr						kW
			N2	O2	H2O	NH3	NO	NO2	
2	7	5.5				10679.8			-174
3	76	5.5				10679.8			279.6
4	170	3.5	126152.7	38311.2		10679.8			7657.6
5	840	3.3	126504	13627.8	16946.3		18064.4		47259.7
6	763	3.3	126504	13627.8	16946.3		18064.4		42495.6
7	592	3.3	126504	13627.8	16946.3		18064.4		31994.6
8	325	3.3	126504	13627.8	16946.3		18064.4		16466.1
9	135	3.16	126504	11412.3	16946.3		13909.6	6370.4	5842.8
10	50	3.16	126504	3995.3	931		1538.6	20616.1	1030
11	20	1	141519	42993					-278
12	184	3.5	141519	42993					8272
13	184	3.5	126152.7	38311.2					7378
14	184	3.5	15366.3	4681.8					894
15	103.5	3.5	15366.3	4681.8					440.4
16	67	3	15366.3	4681.8					233.6
17	52	3	141870.3	8677.1	931		1538.6	20616.1	1267.8
18	224.5	10.25	141870.3	8677.1	931		1538.6	20616.1	9823
19	236	10.25	141870.3	8172.8	931		592.9	22066	10380.5
20	156	10.25	141870.3	8172.8	931		592.9	22066	6377
21	43	10.25	141870.3	8172.8	931		592.9	22066	713.7
22	18	8.9	141870.3	3877	383		15	23	-491.9
23	297	8.9	141870.3	3877	383		15	23	11766.6
24	536	8.9	141870.3	3877	383		15	23	22267.7
25	243	1	141870.3	3877	383		15	23	9237.7
			H2O	HNO3					
26	50	3.16	15078	6462					457.1
27	41	3	36013.4	37865					907.1
28	45	3	36013.4	37865					1114
			H2O(L)	H2O(G)					
29	20	10	24678						-143.3
30	20	80	30036						2604.8
31	194	80	30036						6050.6
32	295	80	38794.3						13063
33	295	80		38794.3					28591.4
34	295	80		30036					22136.6
35	473	80		30036					26900.6
37	50	0.1233	2842.7	27193.3					18865.7
38	50	0.1233	30036						871.8

***Table 10.1** Heat and mass balances of dual pressure nitric acid plant (Gaggioli et al. 1991).*

	Air compressor	NO compressor	Tail gas turbine	Steam turbine

	C1	C2	GT	ST
Isentropic efficiencies	76.0	75.5	81.0	72.0

***Table 10.2** Isentropic efficiencies calculated from Table 10.1. Steam turbine efficiency includes wetness and exhaust end losses which are assumed constant and independent of final moisture content in the steam turbine*

With the energy targeting procedure from pinch analysis it is possible to predict the minimum energy consumption for a given heat recovery problem under the assumption that all streams are known a priori. The energy targeting, however, has little meaning in the case of the nitric acid process because no additional heat supply is desirable. The targeting procedure can instead be used to determine the minimum heat recovery approach temperature. For the base case the minimum approach temperature is found to be approximately 57 °C. A way to utilise the targeting method in Pinch Analysis is to remove all internal heat exchangers and replace them with utility heaters and coolers. This gives a simplified conceptual simulation model (Figure 10.2).

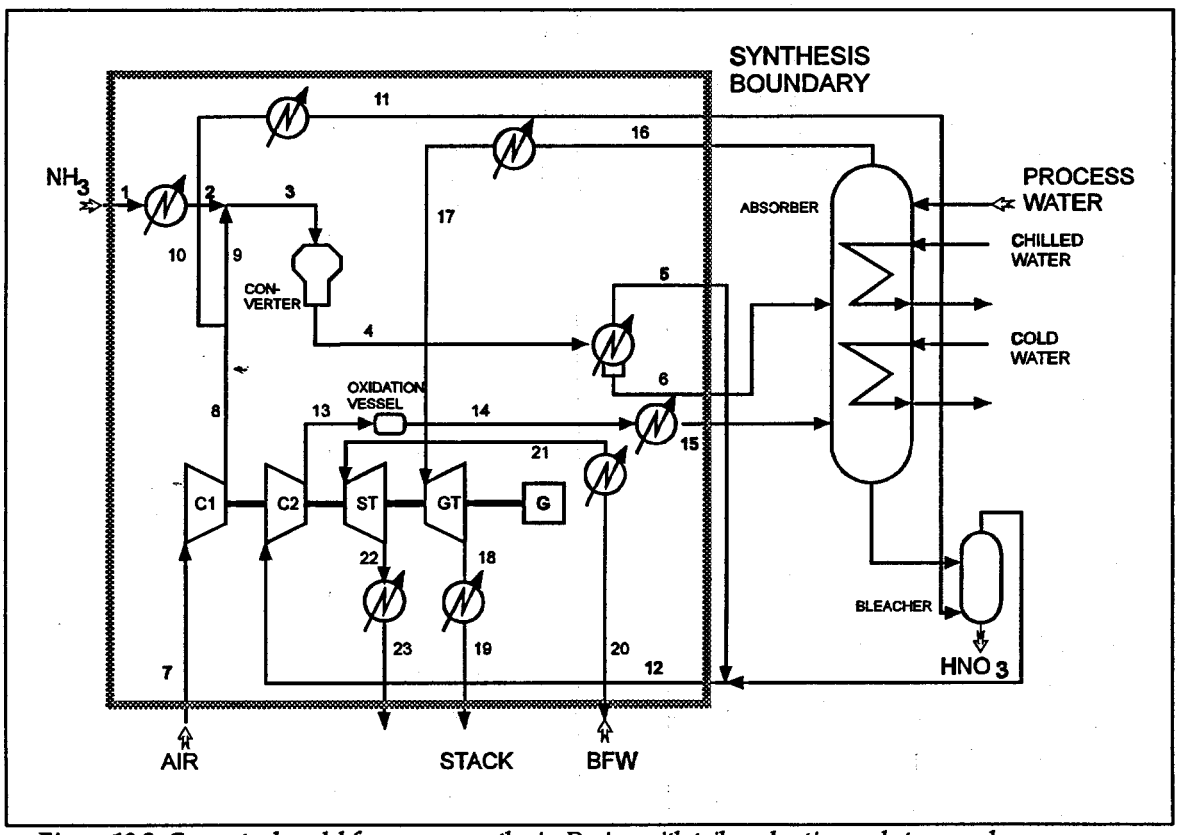


***Figure 10.2.** Conceptual model for process synthesis. Design with tail gas heating and steam cycle.*

With the conceptual model it is possible to write down a strategy for power production improvement which in its general form can be written as

1. Change power related streams (steam flow rate, tail gas temperature etc.).
2. Check that the process to process heat transfer is feasible and obtain minimum approach temperature.
3. Repeat 1 and 2 until a sufficient approach temperature is found.

With this simple strategy it is very simple to evaluate the different options. The simulator gives the resulting power output while the pinch targeting will check for feasibility. The composite curves can be used to identify exergy improvement direction. There is at this stage no need to design the actual heat exchanger network.

In the targeting part it has been decided to use 20 °C and 40 °C as minimum temperature approaches. The above approach has been used to find the optimal power production using the following options.

Tail gas temperature	500 - 700 °C (750 °C)
Steam pressure	80 - 100 bar
Steam flow	free

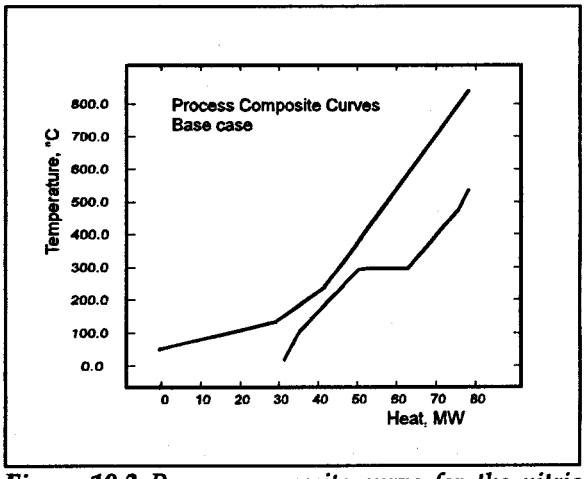


***Figure 10.3** Process composite curve for the nitric acid base case as given by Linnhoff and Alanis (1991).*

A look at the process composite curve (Figure 10.3) for the base case discloses a clear potential for both a tail gas temperature rise and/or a steam increase.

It has been chosen to limit the tail gas temperature to 700 °C in this study. It is, however, easy to evaluate the effect of this constraint using the proposed strategy. The result of several configurations are listed in Table 10.3. From the targeting/simulation result it can be concluded that the best configuration is with maximum tail gas temperature and maximum steam pressure. With the limit set in this study this gives an optimal conceptual design with a tail gas temperature at 700 °C and a steam cycle with a flow rate of 28,641 kg/h (ΔT_{min} = 20°C) and 100 bar. A process with these design values will give a power output of 6492 kW (174 kWh/ton). It can be noted that if we relax the constraint on the tail gas temperature to 750°C, the process will be able to deliver 6952 kW (186 kWh/ton).

No	Tail gas	Steam		Power output	ΔT_{min}
	Temp. °C	Pressure bar	flow kg/h	kW	°C
Base Case	536	80	30036	3971	57.3
A1	600	100	35200	5534	19.7
A2	600	100	32000	4756	40.3
A3	650	100	33700	6011	19.8
A4	650	100	29900	5088	40.0
A5	700	100	32200	6492	19.7
A6	700	100	26250	5046	40.2
A7	750	100	30600	6952	19.9
A8	750	100	24600	5494	39.8

Table 10.3 Performance of optimised conventional process cycle.

10.3 Improved exergy efficiency with tail gas saturation.

A major source of exergy loss in the nitric acid plant is the excessive temperature driving forces at the high temperature level. Even when the tail gas temperature and the steam rising are optimised, there are considerable driving forces (Figure 10.4). The driving forces could be decreased by increasing the massflow of the heated tail gas. In this work it is proposed to saturate the tail gas leaving the absorption column using heated water. The effect of saturating the gas with hot water is twofold - an increase of the massflow and an increased temperature. The higher temperature and flow of the water the higher mass transfer. This is quantified in Figure 10.5 where the tail gas is saturated using an absorption column model.

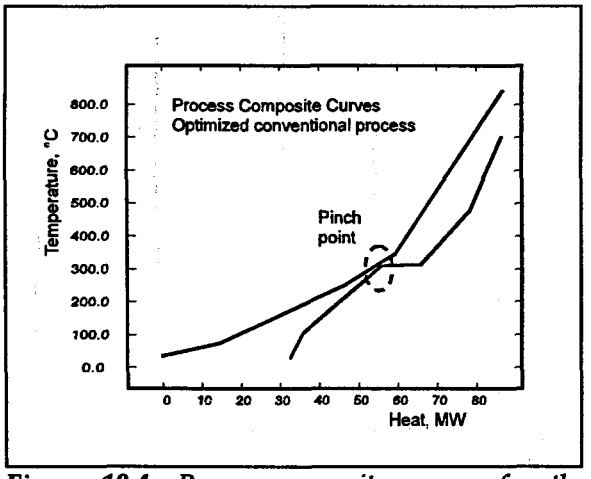


***Figure 10.4.** Process composite curves for the optimised case with the standard process.*

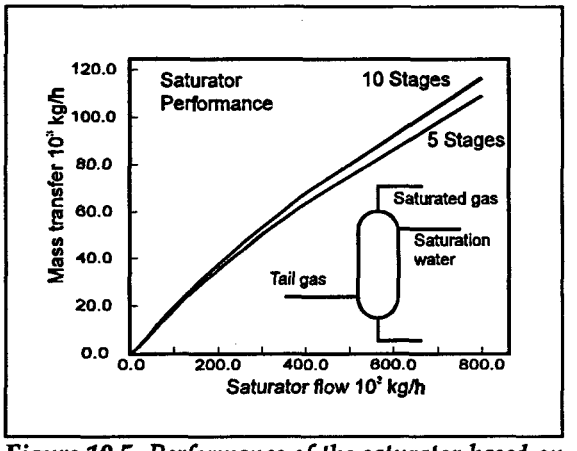


***Figure 10.5.** Performance of the saturator based on 180 °C water. The flow of the tail gas is 146,168.3 kg/h.*

Using the properties for the tail gas in Table 10.1, the performance of the saturator is simulated using HYSIM process simulation software. It is possible to double the total flow of the tail gas if enough hot water is used. The hot water must be produced using the heat from the process. To avoid exergy loss the heating is done in two steps. The fresh water is heated to the saturator outlet temperature and then mixed with the water leaving the saturator. Finally the total water flow is heated to the inlet condition. The saturator can be integrated with the process using the same strategy as before. We assume that all heating demand is handled with hot utilities and all cooling demands with cold utilities. This gives a new conceptual model of the process which is shown in Figure 10.6. It can be noticed that the steam cycle has been removed.

The key parameters for optimisation are in this case:

- Saturator water flow
- Saturator water temperature
- Tail gas temperature

The maximum temperature of the saturation water is set to 180 °C. This limit is chosen to be reasonable working with a saturation water cycle on 12 bar.

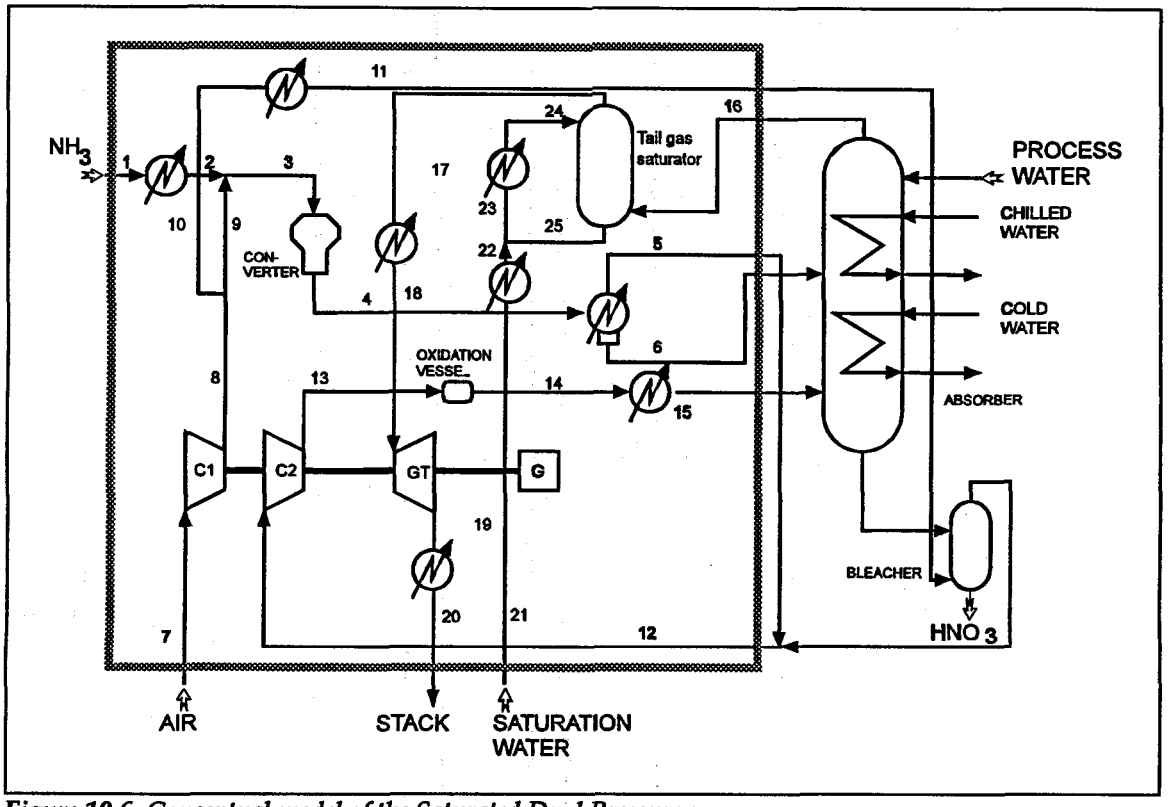


Figure 10.6. Conceptual model of the Saturated Dual Pressure process.

10.3.1 Targeting method for tail gas saturator.

The conceptual model (Figure 10.6) can be simplified further by using a targeting method for tail gas saturation. In the saturation tower a simultaneous mass and heat transfer take place. The associated heat is delivered from the process to the two water heaters. These heaters represent the heat necessary for the saturator. An alternative model could be used to represent the heating requirement. In that model a given amount of fresh water is mixed with the tail gas giving a two-phase flow. The mixture is the heated to the gas turbine temperature. The water gradually evaporates until all water is evaporated. The modified conceptual model is outlined in Figure 10.7. The heat curve for the resulting tail gas/water heater is shown in Figure 10.8. The benefit in using this alternative model is a simplification in the synthesis. In the original formulation it is necessary to include a model of the absorption process. With the new formulation the absorption process and heating of tail gas and water is combined in a simple model where water and tail gas are mixed and subsequently heated. With the new formulation only water flow rate (absorbed) and tail gas temperature has to be specified.

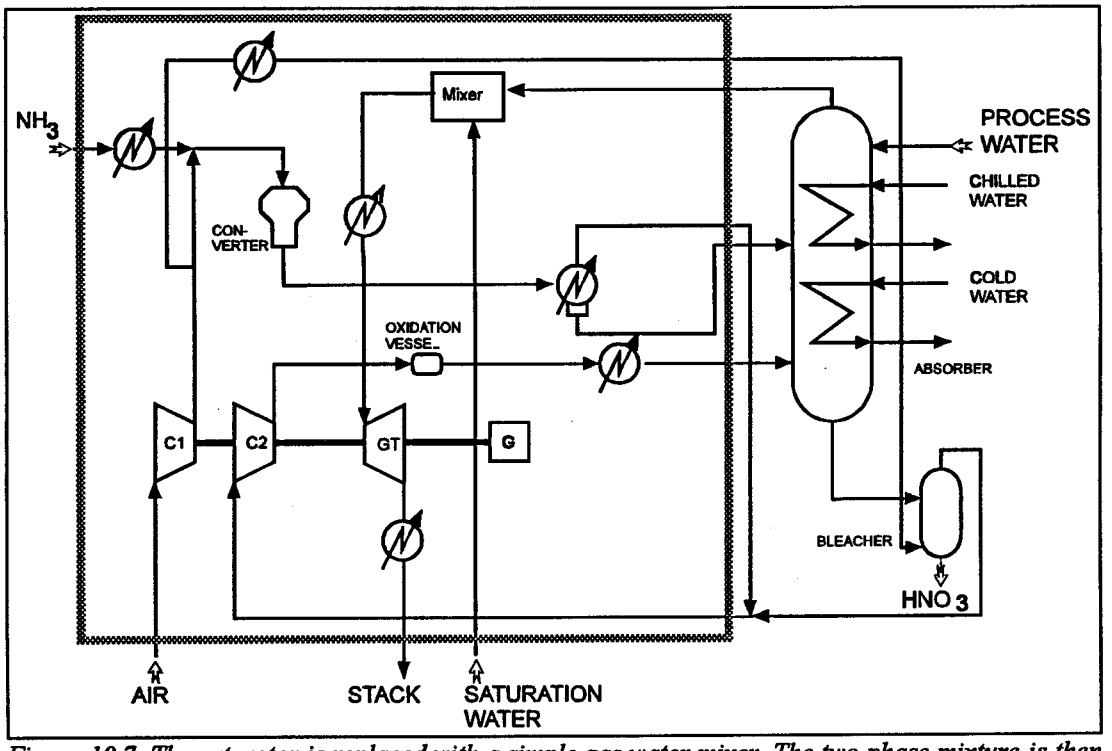


Figure 10.7 The saturator is replaced with a simple gas-water mixer. The two phase mixture is then heated with gradually evaporation of the water.

It is quite simple to retrieve the full model from the targeting model. This can be done graphically - Figure 10.8. The slope of the fresh water heating is determined by the amount of fresh water. The best heating of the rest can be determined by looking at the saturation curve along with the process heat release curve. If the pinch is located at the saturation curve the line has to be drawn through the pinch point in order to maintain the minimum approach temperature.

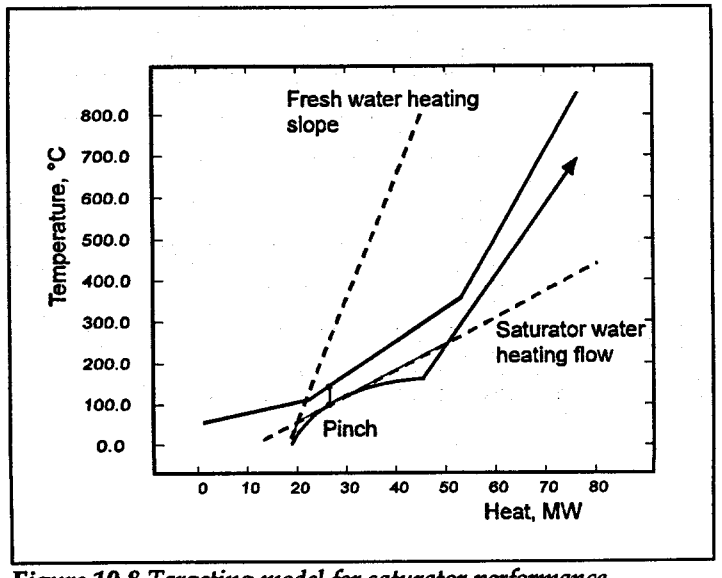


***Figure 10.8** Targeting model for saturator performance.*

10.3.2 Performance of the Saturated Nitric Acid Process.

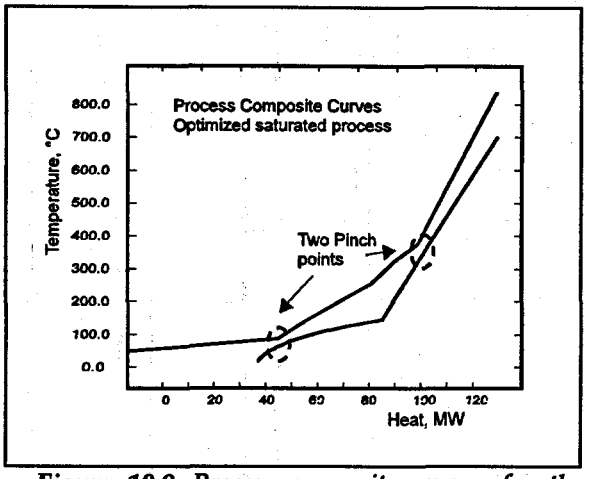


Figure 10.9 Process composite curves for the optimised saturated process.

The proposed modified nitric acid process is optimised using the conceptual model with saturator targeting. The results are, as for the conventional process, obtained with 20 °C as well as 40 °C. With the conceptual model the degree of freedom is cut down to two - tail gas temperature and added water flow. It is thus straight forward to optimise the process iteratively using a standard process simulator (HYSIM). In this case the optimum amount of water is found for a range of fixed turbine inlet temperatures. The results are given in Table 10.4. An interesting feature of the new process is that it exhibits an optimum tail gas temperature at 700 °C. There is in this case no benefit in relaxing the temperature constraint. With ΔT_{min} at 20 °C the proposed process yields 8612 kW (230 kWh/ton) which is 33% better than the optimised conventional process.

Case	Turbine inlet temperature °C	Saturator mass transfer kg/h	Power output kW	ΔT_{min} °C
B1	600	59400	6370	20.3
B2	600	55000	5676	40.2
B3	650	57700	7505	20.3
B4	650	53400	6786	40.0
B5	700	56000	8612	20.4
B6	700	51800	7868	40.1
B7	750	44000	7765	20.1
B8	750	38000	6643	39.9

Table 10.4 Performance of the optimised Saturated Nitric Acid Process

10.3.3 Further improvements?

So far the optimisation has been done in a practical spirit. The technology in the new process is from an economic point of view competitive with the traditional process. In the new process an absorption column and additional heat transfer equipment replace the steam turbine which is a high capital cost equipment.

An alternative to the Saturated process is a process with more than one steam pressure. As a practical extreme we have chosen to optimise the plant using three steam pressure levels (100, 12 and 1 bar) with associated steam turbines. With the same conditions for the core process (Table 10.1) this gives a net power output of 8819 kW (235 kW/t(HNO_3) at ΔT_{min}=20°C.

It is also possible to boost the Saturated Process by including a steam cycle. The extended Saturated Process is optimised using an 100 bar steam cycle. The results are given in Table 10.5. With the 700 °C constraint on turbine temperature a new optimal power production is found to 9778 kW (261 kWh/ton) with ΔT_{min} = 20°C. For each gas turbine inlet temperature the optimum configuration is found when two pinches occur simultaneously. One pinch caused by the steam raising and one by the saturation water heating.

Case	Turbine temperature °C	Saturator mass transfer kg/h	Steam production kg/h	Power output KW	ΔT_{min}
C1	600	34500	24500	8395	19.7
C2	600	34900	22000	7519	40.0
C3	650	37000	20600	9045	19.7
C4	650	39500	15300	7944	39.8
C5	700	37500	19500	9778	20.0
C6	700	42000	9500	8440	39.7
C7	750	38000	17000	10518	19.9
C8	750	33000	18500	9257	40.4

***Table 10.5** Performance of the extended Saturated Nitric Acid Process.*

The extended Saturated Process thus delivers about 11 % more power than the multi steam pressure process. The estimated equipment cost will probably be considerable lower for the new process compared with the multi steam level process.

10.3.4 Heat exchanger network design

Until now all evaluations have been done at a conceptual level, not taking into account the specific heat exchanger network. It has been assumed that a minimum approach temperature should be maintained. This value should represent the correct energy capital trade-off.

To investigate the difference in heat exchanger network design among the concepts, two networks will be designed. One for case A5 and one for case B5. The networks are synthesised with *HEN Explorer* (see chapter 6). It is assumed that the cost function follows:

$$Installed\ Cost = 4000\ Area^{0.6}\ [US\$]$$

The resulting networks are shown in Figure 10.10.

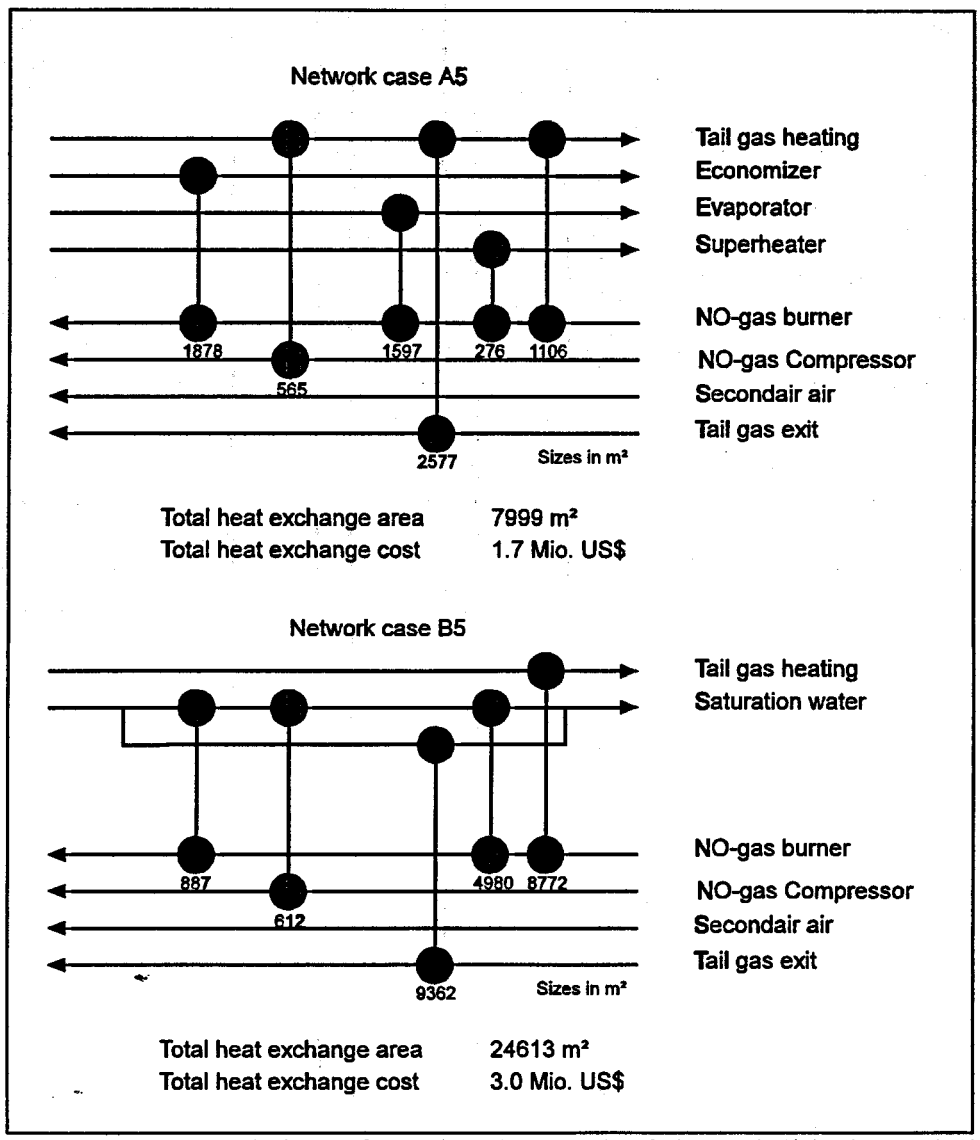


Figure 10.10 *Network design for optimised conventional design (A5) and optimised saturated design (B5).*

The additional heat exchanger cost for the saturated process compared with the conventional process is thus 1.3 10^6 US$. Compared with the huge increase in power output and the fact that the steam turbine is removed this additional cost seems to be quite small.

10.3.5 Turbo machinery efficiencies

For comparison the different process concept has been evaluated for the same equipment efficiencies as imposed by table 10.2. These efficiencies are, however, lower than those available for new plant design. Better understanding and advanced aerothermodynamic modelling of compressors and expanders have lead to a dramatic increase in turbo machinery within the last decades. Modern gas turbine system thus operates with *polytropic efficiencies* for compressors of approximately 88% to 91% and for expanders 83% to 88%.

For the steam turbines used in this study the adiabatic efficiency of 72% seems to match reasonably with the values of those machineries delivered in the last decade or so. Under the conditions used in this study a typical exhaust end loss and moisture loss will each be approximately 2.5%. When the steam turbine is downsized, as with the boosted saturated cycle, these losses will increase. Therefore, in that particular case a reasonable adiabatic efficiency will be approximately 67%.

To see the effect of increasing efficiency optimisation has been carried out with the adiabatic efficiencies given in Table 10.6.

	Air compressor C1	NO compressor C2	Tail gas turbine GT	Steam turbine ST
Polytropic efficiency	89	86	85	
Isentropic efficiency	87	83	88	72.0[1]

***Table 10.6** Updated turbo machinery efficiencies.*

With these values the optimisation can be revised, which is done for maximum gas turbine inlet temperature (700°C) and ΔT_{min}=20°C (Table 10.7).

Gross power output kW	Conventional design A5	Saturated design B5	Multi steam level design	Enhanced saturated design C5
Table 10.2 efficiencies	6492	8612	8819	9778
Table 10.6 efficiencies	8679	11826	10927	12341

***Table 10.7** Effect of using state of the art efficiencies.*

10.4 Integration of the saturated process in Kemira unit IV.

The above sections have demonstrated an enhancement of the energy efficiency by saturating the tail gas. So far only new plant design has been considered. In this sub section the possibilities of boosting Kemiras HNO_3 unit IV with tail gas saturation are evaluated.

[1] 72% for large steam flow and 67% for small steam flow.

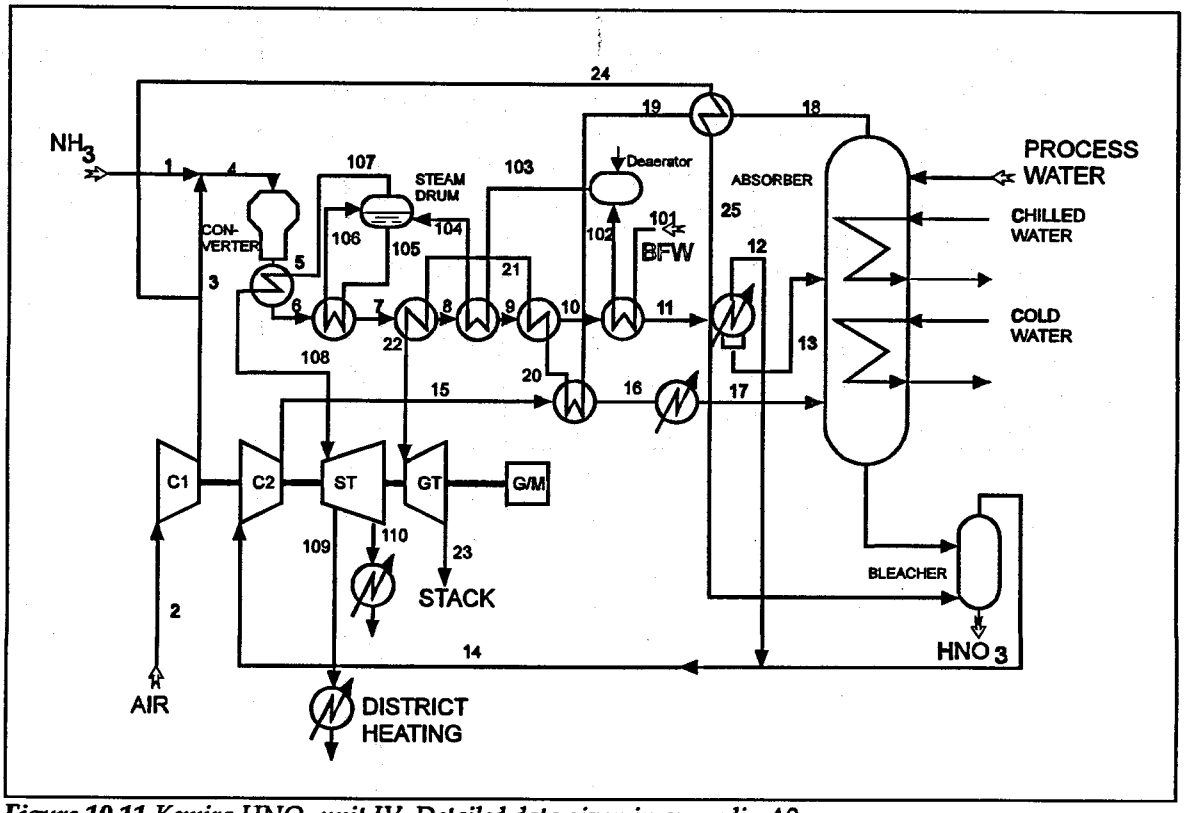


Figure 10.11 Kemira HNO_3 unit IV. Detailed data given in appendix A2.

Process data for Kemira HNO_3 unit IV (Figure 10.11) is given in appendix A2. The first step is to evaluate the potential improvement. Only small changes in process parameters will be accepted. One problem with additional tail gas flow is the enhanced pressure drop, which will influence on the operation point of the turbo machinery. A practical constraint chosen is, that the additional flow must not exceed 5% of the original tail gas mass flow rate. This gives a maximum mass transfer of 5400 kg/h. Further the tail gas temperature must not exceed 350°C.

Case	Mass Transfer kg/h	Tail gas temperature °C	ΔT_{min} °C	Power output kW
Base	0	320	53.3	3595
A1	2000	320	50.0	3824
A2	4000	320	46.9	4053
A3	6000	320	36.5	4282
A4	8000	320	21.1	4511
B1	2000	340	41.1	4094
B2	4000	340	37.8	4331
B3	6000	340	28.8	4568
B4	8000	340	15.3	4805

***Table 10.8** Targeting analysis for integration of Sat Cycle.*

The approach proposed in the above sub section, is used for targeting for improved power generation. The steam generation will be kept fixed in the targeting analysis. A

specified amount of water is mixed with the tail gas and heated to a specified temperature. Based on values for these two parameters the resulting power output is calculated in HYSIM and a pinch analysis gives the resulting ΔT_{min}. The results for tail gas temperature of 320 and 340 are given in Table 10.8.

The potential savings are thus in the range of 500 to 1000 kW. The plant operates about 7500 h/yr. With an expected electricity cost of 0.3 DKK/kWh the savings will be 1.1 to 2.2 MDKK/yr.

High capital cost is associated when modification is made of the existing heat exchanger network. It is therefore crucial to keep the number of alternation at low level, to get a successful retrofit.

When operating in district heating mode, the feed water temperature is typical 100°C. This results in a low efficiency of the low pressure economisers. The district heating condensate could instead be used in a new tail gas absorber placed after the existing absorption tower. Other heat sources could also be considered.

An off-design model of the heat exchanger network is established (appendix A2). This model can be used to evaluate the effect of humidifying the tail gas. HYSIM's absorber column model is used to simulate the humidification of the tail gas using a 10 stages column. The model predicts the resulting changes in temperatures throughout the HEN. The economiser temperatures are affected and it is necessary to correct the steam production accordingly. This is done by calculating the missing heat effect in the economisers and thus compensate for this, by reducing the produced steam flow rate.

In Table 10.9 the results of varying the saturator water flows are given.

Case	Saturation flow kg/h	Mass Transfer kg/h	Tail gas temperature °C	Uncorrected power kW	Losses steam turbine kW	Power output kW
Base	0	0	320	3592	0	3592
1	5000	200	319.7	3614	-7	3621
2	10000	449	319.7	3642	-14	3656
3	15000	760	319.5	3675	-17	3692
4	20000	1121	319.1	3712	-17	3729
6	30000	1925	318.2	3792	-17	3809
7	40000	2715	317.2	3869	-14	3883
8	50000	3430	316.3	3937	-10	3947
9	100000	5875	313.0	4169	7	4162

***Table 10.9** Off design results integrated Sat Cycle.*

It is interesting to notice that saturation of the tailgas has very little effect on the economisers. Actually the feed water temperature out of the high pressure economiser is within 1°C of the original value. The feed water temperature out of the low pressure economiser is in the range 0°C to 5°C above the original value. This gives a minor reduction in 4 bar steam usage.

The possibility of enlarging one of the existing exchangers has been evaluated. The results are summarised in Table 10.10. A saturator flow of 30000 kg/h has been used.

Case	new UA kW/K	Tail gas temperature °C	HP economiser temperature °C	Uncorrected power kW	Loses steam turbine kW	Power output kW
Changes in the final tail gas heater (Ex1) - Original UA = 72.29 kW/K (968 m²)						
	80 (1071)	322.9	198.4	3855	28	3827
	100 (1339)	332.6	193.0	3985	120	3865
	120 (1606)	339.8	189.0	4083	189	3894
	140 (1875)	345.3	185.9	4157	242	3915
	160 (2142)	349.6	183.4	4216	285	3931
	180 (2410)	353.1	181.4	4262	320	3942
	200 (2678)	355.9	179.8	4300	347	3953
	300 (4017)	363.9	175.2	4366	396	3970
	500 (6695)	368.7	172.4	4474	475	3999
Changes in the second last tail gas heater (Ex3) - Original UA = 41.24 kW/K (507 m²)						
	50 (614)	319.3	202.4	3807	-41	3848
	60 (737)	320.4	203.6	3821	-62	3883
	70 (860)	321.2	204.7	3832	-81	3913
	80 (983)	322.0	205.6	3842	-96	3938
	90 (1106)	322.6	206.4	3850	-110	3960
	100 (1228)	323.1	207.0	3858	-120	3978
Changes in the second tail gas heater (Ex6) Original UA = 29.84 kW/K (237.7 m²)						
	40 (319)	318.9	201.8	3801	-31	3832
	50 (398)	319.4	202.5	3808	-43	3851
	60 (478)	319.8	202.9	3814	-50	3864
	70 (558)	320.1	203.4	3817	-58	3875
	80 (637)	320.4	203.7	3821	-64	3895

***Table 10.10** Off design results - integrated Sat Cycle with additional heat exchange area.*

The results in Table 10.10 shows that additional 100 kW can be expected if the size of either exchanger Ex1 or Ex3 are enlarged to about double size. This does not seem to be an attractive solution. However, if one of exchangers has to be replaced then it might pay off.

The pressure drop in the new absorber and due to increased flow, also has to be considered. If a pressure drop in the absorber is assumed 0.1 bar and the increased pressure drop due to increased flow is 0.03 bar, the resulting loss in the expansion can be calculated to approximately 40 kW.

Consequently an improvement of approximately 170 kW in shaft power output can be expected with no additional heat exchange surface and approximately 310 kW can be expected with a doubling of heat exchange area for either of Ex1 or Ex3. The analysis has assumed that water at 100 °C is available in sufficient amount.

10.5 Conclusion and significance - Nitric acid energy synthesis.

This chapter has demonstrated how a top down analysis of a given process can give considerable improvements in energy efficiency. By using a structured approach that takes advantages of different design technologies (Heuristics, Exergy, Pinch and mathematical methods) a new concept for energy efficient nitric acid production has been evaluated and optimised. This has resulted in an improvement in specific power production from 171 kWh/t(HNO_3) to 258 kWh/t(HNO_3) using conservative equipment efficiencies as imposed by Linnhoff and Alanis (1991).

Using more appropriate turbo machinery, it has been shown that the proposed saturated nitric acid process is able to produce nitric acid giving a gross power output of 312 kWh/t(HNO_3) with no steam cycle and up to 326 kWh/t(HNO_3) with a small additional steam cycle.

Considering that today's nitric acid plants have a typical power output in the range 0 to 140 kWh/t(HNO_3), the new process has a good change of ousting the conventional nitric acid process, when it comes to new design.

With regard to integration of the saturated process into the existing plant HNO_3 IV at Kemira improvement is only possible with considerable associated costs. This is mainly due to the high degree of integration in the current plant and the fact that the expander here operates at low temperature.

11
ENERGY SYNTHESIS OF THE SULPHURIC ACID PROCESS

In this chapter the Sulphuric Acid process will be evaluated in terms of energy efficiency. Optimisation of energy utilisation is carried out for the conventional double absorption process as well as a pressure contact process. This is done by using the general approach for conceptual optimisation discussed in chapter 7.

The analysis will only treat new plant design.

11.1 Commercial sulphuric acid production.

Sulphuric acid is one of the most important chemicals in the heavy industry. It's used in a wide range of industries. These industries include petroleum refining, pigment production, plastic industry and fertiliser industry.

Actually enough sulphuric acid is contained, in exhaust gases from combustion of coal, oil and other sulphur containing fuels, to supply the worlds sulphuric acid needs. Until recently it has not been economical to replace the traditional sulphuric acid methods. Recent changes in environmental regulations have however changed this and today operating fluegas cleaning systems produce commercial sulphuric acid.

Even though the time of the sulphuric acid plants based on elementary sulphur seems to be limited there is vast number of operating plants. Further the sulphuric acid production based on flue gas is still only economical with strong legal regulations. Therefore the sulphuric acid industry certainly will continue for some years on.

Sulphuric acid production from elemental sulphur is in principle carried out in three steps. First the elemental sulphur is oxidised producing sulphurdioxide. Secondly the sulphur-dioxide is further oxidised forming sulphur trioxide. And finally the sulphurtrioxide is absorbed in sulphuric acid and reacts with added water to form more sulphuric acid.

All tree steps are exothermal and the reactions take places in accordance with equation (11.1) to (11.3).

$$S(rhomb) + O_2\,(g) \rightarrow SO_2 \quad \Delta H = -297\,kJ/mol \tag{11.1}$$

$$SO_2\,(g) + 0.5\,O_2 \_ SO_3 \quad \Delta H = -99.0\,kJ/mol \tag{11.2}$$

$$SO_3\,(g) + H_2O\,(l) \_ H_2SO_4\,(l) \quad \Delta H = -132.5\,kJ/mol \tag{11.3}$$

11.2 Case study - Double Absorption process.

The base case used in this study is Kemiras existing plant, which is a Sulphur-Burning Double Absorption Sulphuric Acid Process (Lurgi design). The process lay out is shown in Figure 11.1.

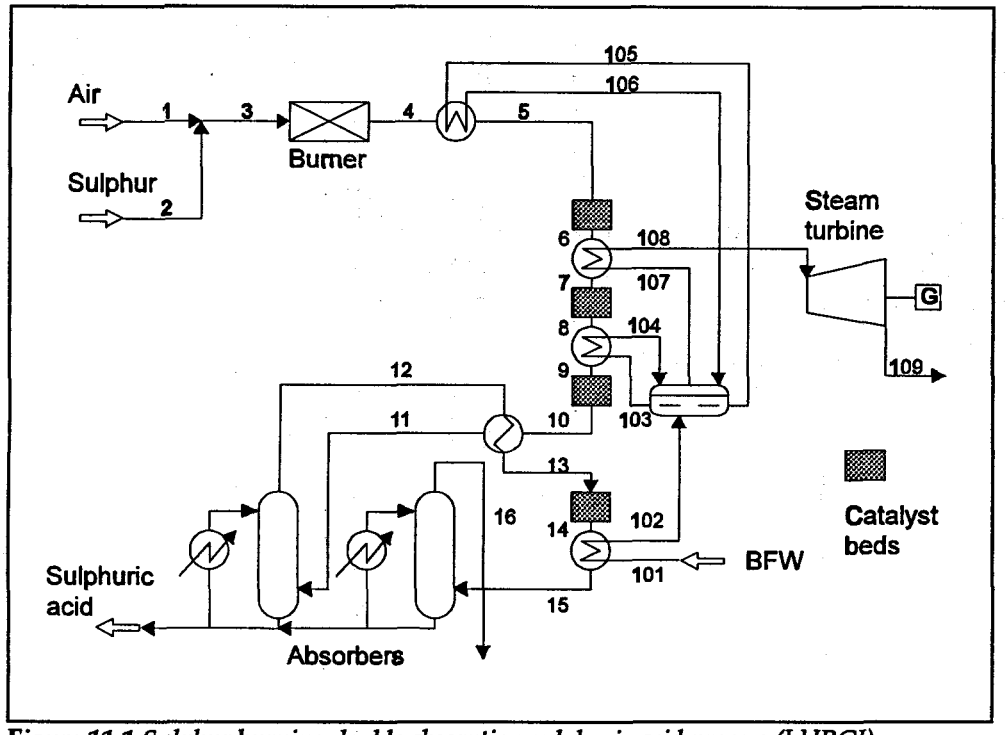


Figure 11.1 Sulphur burning double absorption sulphuric acid process (LURGI).

The steam turbine (BBC) is an extraction back pressure turbine. The extraction steam (9 bar) and back pressure steam (4 bar) is delivered to the site steam mains. It is thus the steam usage at site that determines the plant operation. Surplus or deficit in steam production can be exported/imported from the high pressure steam main.

To evaluate the general performance of the sulphuric acid plant minor changes have been made for comparison among process alternatives. It is thus assumed that the high pressure steam is operating as a condensing turbine. In that way the energy efficiency can conveniently be expressed by the net power production. The case study in this chapter can thus be considered as a power producing version of Kemiras sulphuric acid plant. Based on the information available from the supplier, the mass and energy balances have been established. The data are found in appendix A3. The objective for the study is to maximise power production for $\Delta T_{min} = 20$ °C. The steam turbine isentropic efficiency is set to 72% which seems to be reasonable for a modern unit working under the specified conditions.

The procedure outlined in chapter 7 is as follows

1. Obtain base case configuration.
2. Remove all utility streams (non kernel process streams) - Conceptual model.
3. Select basic utility concept(s).

4. Set initial/Update kernel process parameters and key utility parameters.
5. Serve all process streams with simple utilities (coolers and heaters).
6. Calculate pinch targets (minimum energy use based on ΔT_{min} or minimum approach temperature in threshold problems).
7. Repeat step 4-6 while optimising energy recovery, material conversion or power production.
8. Design heat exchanger network for optimised process and utility concept.

In this case study the synthesis will stop at step 7.

Base case configuration is given in Figure 11.1. The conceptual model (Step 2) is outlined in Figure 11.2. In the conceptual model the utility concept is imposed in form of a steam cycle. In the initial study a steam cycle at varying pressures will be examined (step 3). With a given steam pressure an initial steam flow rate is chosen. With a given steam pressure and flow rate the resulting power output can be calculated using the conceptual model. The steam heating is in the conceptual model served by an external heater that heats the boiler feed water from its initial condition to its destination conditions (step 5). With all streams associated with an external utility a pinch analysis can be used for targeting a ΔT_{min} (step 6). Since no heat should be added this problem can be considered to be a threshold problem. If the targeting gives a $\Delta T_{min} < 0$ then a heat exchanger network will be unable to meet all heating demands and the process thus infeasible. In this study a minimum ΔT_{min} that is accepted is 20°C. If $\Delta T_{min} > 20$°C then the steam flow rate can be increased and a new targeting analysis can be made. This is continued until $\Delta T_{min} = 20$°C is reached (step 7).

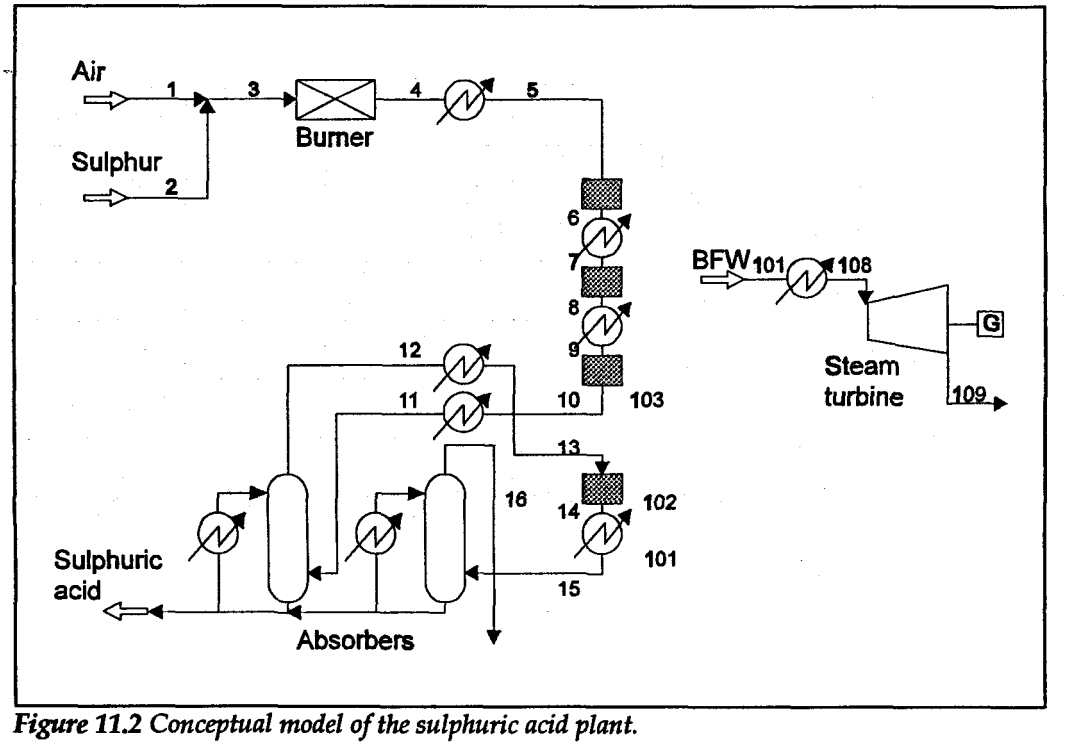


Figure 11.2 Conceptual model of the sulphuric acid plant.

For a steam pressure of 43 bar (existing pressure level) the results will be as follow (Table 11.1).

Table 11.1 Steam production 43 bar Steam flow kg/h	Power output kW	ΔT_{min} °C
38000 (base case)	8265	52.8
40000	8700	29.5
40860	8890	20.0
41000	8917	18.5
42000	9135	7.9

The power output of the base case design can thus under the given constraints be improved by 625 kW by increasing the steam production. The power improvement will come at the cost of increased heat exchange area due to the decreased heat transfer driving forces.

An obvious way to increase the power production is to increase the steam pressure. A maximum steam pressure is set to 100 bar which should reflect an industrially practical steam pressure limit. The same conceptual model as before can be used for the analyses and the results are given in table 11.2.

Table 11.2 Steam production 100 bar Steam flow kg/h	Power output kW	ΔT_{min} °C
36000	9037	63.6
38000	9539	38.1
39000	9790	26.1
39500	9916	20.4
40000	10041	14.6

The power production can thus be increased by another 1000 kW to 9916 kW by increasing the steam pressure.

11.3 Pressure contact process.

A variant of the double absorption process is the pressure contact process (Cameron et al. 1978), where the process is carried out under pressure. This process has several advantages over the conventional process. First of all the sizes of the converter, absorption towers and pipes will be reduced. This could represent a major cost saving. Further the chemical equilibrium of sulphur dioxide will be more favourable at high pressure (Sander et al. 1984). This will result in higher conversion rate.

The principal disadvantage of the pressure process is according to Sander et al. (1984) that the process consumes more power and produces less steam. This is, however, not quantified. The purpose of this section is to investigate if the pressure contact can be made competitive in energy efficiency compared with the conventional process.

Only limited data are available for the pressure contact process. In the case study here it is assumed that the conversions are the same as for the atmospheric process. This is according to the above a conservative assumption.

The combustion air is in the case study model compressed. The combusted gas then follows the same path as in the atmospheric process to the end absorber. The tail gas leaving the absorption tower is finally expanded in a tail gas turbine.

The conceptual model of the pressure contact process is outlined in Figure 11.3. In the model the compression is done in two stages with an intercooler. The pressure losses are assumed proportional to the discharge pressure of the two compressors (2% in intercooler and 7% between the second compressor and the expander). Efficiencies for the two compressors are set to 87% and 83% respectively and 88% for the expander.

The intercooler cools the temperature into the second turbine to 40 °C. A constraint of 700°C for the tail gas temperature is imposed. The pressure ratios for the two compressors are varied independently. This is, however, kept in mind that optimum performance for intercooled compressors normally requires that the two pressure ratios are almost equal. In this case with higher efficiency and lower inlet temperature for the first compressor it must be expected that the pressure ratio of the first compressor is slightly higher than for the second.

In an initial study the discharge pressures have been fixed at 3 bar and 8 bar. The resulting pressure ratios are thus 3 and 2.7. The results are outlined in table 11.3.

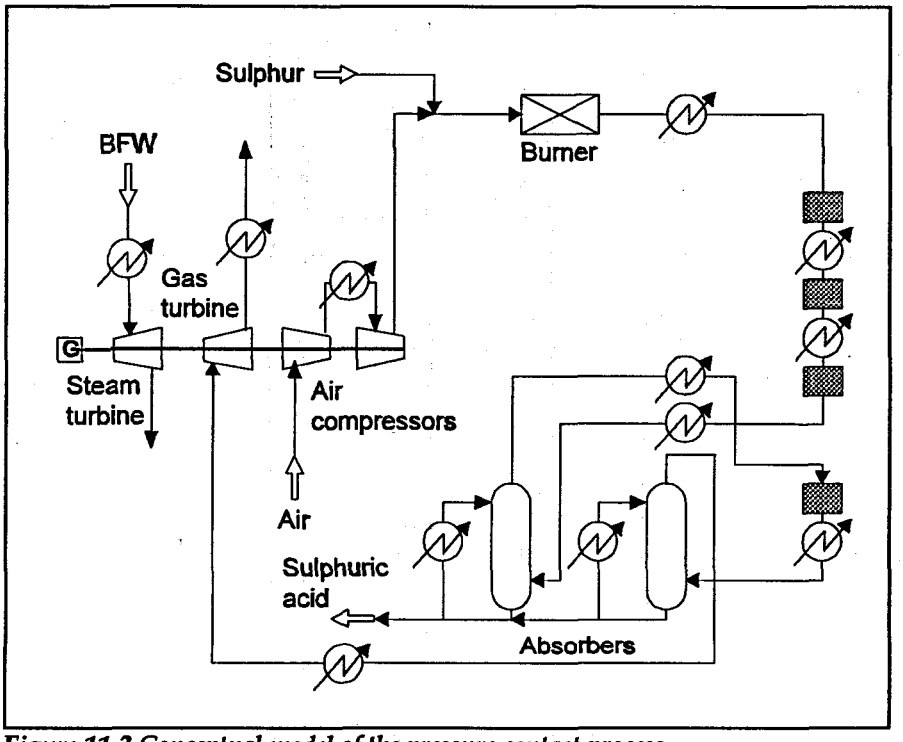


Figure 11.3 Conceptual model of the pressure contact process.

Table 11.3 Pressure contact process Steam kg/h	Power output kW	ΔT_{min} °C
0	1659	368.1
10	4170	159.5
20	6680	178.0
30	9190	50.5
32	9692	29.7
33	9943	19.8

This shows that the pressure contact process has the potential of becoming just as energy efficient as the atmospheric process.

The process composite curve for the optimised pressure contact process (in appendix A3) shows that the pinch is located at 140°C/120°C. The heat released in the intercooler (149.4°C to 40°C) is thus placed under the pinch. If the inlet temperature to the compressor is increased the combustion temperature will increase accordingly. The compressor can thus be regarded as a heat pump working across the pinch. Further improvement could thus be expected if the amount of heat removed from the intercooler is lowered. If the pinch is very distinct an optimum intercooler outlet temperature would be 140°C (pinch temperature). Then the intercooler only retrieves

heat across the pinch and heat under the pinch is heat pumped to above the pinch. It is, however, necessary to check if the pinch moves. An analysis with an intercooler exit temperature of 140°C shows that the pinch does not move. The benefit is an increase in power production from 9943 kW to 10082 kW. This also reduces the pressure necessary heat exchange area and thus the pressure loss.

These considerations have been further confirmed using the targeting method for different intercooler outlet temperatures (Table 11.4). The results show that the optimum indeed is at an intercooler exit temperature of 140°C.

Table 11.4
Effect of decreasing intercooling temperature

Temperature °C	40 (Base)	60	80	100	135	140	149.4
Power output kW	9943	9960	9991	10022	10074	10082	10025

The optimum intercooler temperature is in fact close to the compressor discharge temperature. The amount of heat recovered is therefore little. It would therefore be practical to make the total compression in one step. This would reduce the capital cost of the plant considerably.

11.4 Saturated sulphuric acid process.

A process similar to the saturated nitric acid process (Chapter 10.3) is considered. The tail gas leaving the last sulphuric acid absorber is humidified in an absorption tower. A simplified model based on mixing water and tail gas is used to evaluate the potential of this process (see chapter 10.3). The modified process is evaluated with and without steam cycle.

Optimisation of the process without steam cycle is conducted by selecting a discharge pressure for the first compression stage and the find the optimum discharge pressure for the second compressor with the ΔT_{min} = 20°C constraint. The role of the intercooler discussed in the previous section is not considered in the initial phase.

The amount of water transferred to the tail gas and the resulting power output at different pressure levels is given in table 11.5.

The saturated process is thus not competitive with the dry pressure contact process in energy efficiency.

Table 11.5

Saturated sulphuric acid process - no steam cycle		
Discharge Pressures bar / bar	Water in tail gas kg/h	Power output kW
3 / 7	41500	8775
3 / 8	40500	8958
4 / 12	38100	9224
4 / 14	37200	9324
4 / 15	36850	9326
4 / 16	36550	9320
5 / 18	35100	9178
5 / 20	35400	9210
5 / 22	34900	9155

If the saturated process is enhanced with a steam cycle this could change. The combined process is optimised for a single set of pressure levels (3 bar / 8 bar). This gave a new energy optimal process with the following parameters:

Water content in tail gas	10000 kg/h
Steam production	30500 kg/h
Power output	11124 kW

The pinch is in this case located at 105°C/85°C. Using the principles derived in the previous section the optimal intercooler exit temperature should be 105°C. This change results in small increase in power output and the resulting optimal process with the selected pressures are thus

Water content in tail gas	10000 kg/h
Steam production	32900 kg/h
Power output	11138 kW

11.5 Discussion - Sulphuric acid processes.

In this chapter the energy aspects of sulphuric acid production are discussed. With the falling price for sulphuric acid energy has become one of the principle factors for economical sulphuric acid production. It is thus of importance that the production is done as efficient as possible.

Hitherto, the atmospheric process has been regarded as the most energy efficient process, while the pressure process is preferable for maximum conversion. The studies in this chapter prove that maximum conversion and energy efficiency not necessarily counteract each other. The pressure contact process can thus be optimised

to give a superior efficiency (322 kWh/t(H_2SO_4)) compared with the optimised atmospheric process (292 kWh/t(H_2SO_4)).

A new route to optimal energy efficiency has also been discovered. The new process is based on humidification of the tail gas. With the new concept it is possible to produce sulphuric acid with a power production up to 356 kWh/t(H_2SO_4). This can be compared with the values for the conventional processes that produce 264 kWh/t(H_2SO_4).

An interesting new aspect of compressor integration has been discovered during the study. It has been demonstrated that integrated compressors can be treated as heat pumps during the synthesis.

12
PERFORMANCE CALCULATION AND MONITORING

12.1 Introduction.

Although process design optimisation is an important task - as discussed earlier in this thesis - it is equally important to ensure that the equipment maintains high individual efficiency during operation. Performance monitoring has for long been an overlooked area in process system engineering. It is, however, well known within aircraft industries, where it is of vital importance to detect performance degradation of the propulsion engines. This chapter will only treat the practical aspect of performance monitoring with regard to Kemira. There will thus only shortly be discussed some general aspects on performance monitoring.

From a system engineering point of view, the effect of a units performance degradation should be measured by the effect on the system performance. To illustrate the effect of performance degradation of a simple gas turbine cycle is considered (Figure 12.1).

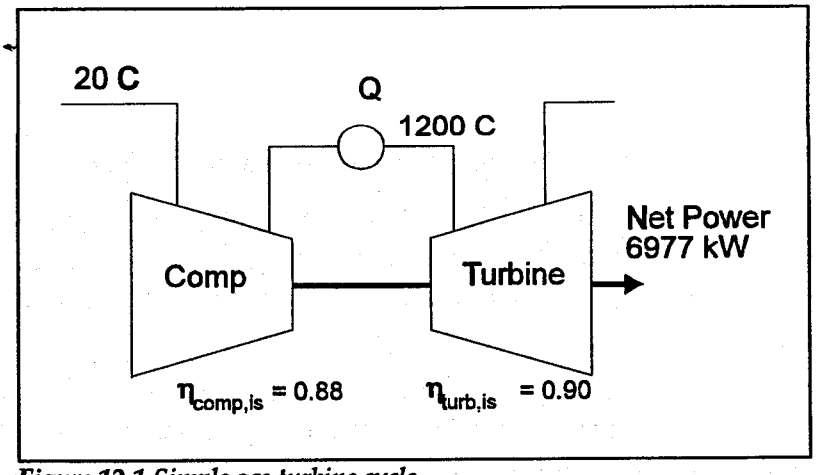


Figure 12.1 Simple gas turbine cycle.

The effect of a performance degradation is evaluated in table 12.1

It is noted that even small changes in unit performance can have major impact on total system performance. This is especially pronounced in systems where energy loads are balanced as in this case via the mechanical shaft. Here the two large power loads are balanced yielding a somehow smaller net output. It is noted that the performance degradation affects both the total efficiency as well as the power production rate. In general degradation will affect both yield efficiency and plant capacity. The worse effect of the two depends closely on the economical aspects of the plant operation. If

the operating costs are small and the capital costs high, then it is most probably that plant capacity is most essential and vice versa.

$\eta_{comp,is}$ %	$\eta_{turb,is}$ %	$\Delta\eta_{is}$ %	Power kW	Heat Q	η_{sys} %	ΔPower %	$\Delta\eta_{sys}$ %
88	90	-	6977	16538	42.19	-	-
87	90	1.1	6863	16424	41.80	1.6	0.9
88	89	1.1	6790	16538	41.06	2.7	2.7

Table 12.1 Effect of performance degradation in simple gas turbine cycle.

In many cases it can be very difficult to detect real performance degradation. Typically the equipment operates away from design conditions. In the gas turbine example, the inlet temperature will normally vary and thus affect the operation. It is therefore in general important to be able to correct the resulting parameter so that the operating values can be compared on a common basis.

In the subsequent chapters (12.2 and 12.3) real cases at Kemira will be discussed. The first case deals with some practical problems that occur regarding measurements and uncertainties. The second case show how simple models can be evolved and used for performance evaluation.

12.2 Performance monitoring - BBC steam turbine.

In conjunction with the Sulphuric Acid plant and connected with the site utility system is the BBC steam turbine. The turbine has been in operation since 1972. It operates with a nominal inlet steam condition of 43.15 bar, 425 °C and has an extraction at 9 bar. The backpressure is 4 bar. In the purchase documentation is a guiding performance characteristic but unfortunately no guaranty points.

The primary instrumentation consists of two flow measurements (live and extraction steam flow rates), two temperature measurements (live steam flow and backpressure steam flow) and finally three pressure measurements (live steam, wheel chamber and extraction).

It has been noted by the operating staff that the turbine for many years has not delivered the power per ton steam as expected from the performance curve. Several measured points are compared with the performance map. This reveal an apparently large deviation between measured and expected performance. The deviation is in the range of 0.6 to 0.8 MW.

There can be several reasons for this apparent deviation:

1. Error's and/or inaccurate measurements.
2. Operation outside normal operation range.
3. Changed operation conditions (live steam, back pressure etc.).
4. Degradation of turbine.

Incorrect measurements

The steam flow measures are all based on measuring over a nozzle. Beside the ordinary inaccuracy there is one obvious error because there has been no correction for actual steam condition. The measurement is based on a conversion from pressure reduction to velocity and then from velocity to massflow based on steam density ρ. In the current configuration the density is calculated as fixed based on the nominal condition

Basis	43.15	bar
	425	°C

while the real condition is in the range

Real condition	37-40	bar
	390-405	°C

The relation between the measured flow rate and the reel flow rate can thus be expected to be

$$\dot{m} = \sqrt{\frac{\rho_{real}}{\rho_{basis}}} \qquad (12.2.1)$$

The density of steam is dependent on pressure as well as temperature. The deviation will under typical conditions be between 2 - 4 %. This deviation will result in an overestimation of the steam flow rate by 0.9 t/h. Taking this into account, the deviation between expected power output and real output is now reduced to 0.5 - 0.7 MW.

Operation outside normal operation range.

The turbine operates at low load. Under low load operation it is normal to have a considerable steam turbine exit loss. This will result in a rise in the steam exit temperature. From the turbine characteristic it is possible to calculate the isentropic efficiency of the steam turbine. With the specific numbers this gives

Flow	η_{is}
t/h	%
40	80
30	78
20	67
18	62

These values are based on a situation with no steam extraction and nominal live steam conditions.

Non nominal steam condition

The performance curve is drawn under the assumption that the live steam is at the nominal condition. As mentioned earlier, the real live steam condition is somehow different. The isentropic expansion at nominal condition give 571.06 KJ/kg(steam) while at f.x. 400 °C, 39 bar 534.43 KJ/kg(steam). It can thus be expected that the turbine output will decrease with approximately 6 %.

Turbine degradation

Unfortunately there is no record on performance for the turbine during the last 20 years. There is thus no way for tracing any degradation. There is however a small risk of deposition on the first rows of blades.

Summary

The revision has revealed following:

Uncorrected steam measuring overestimates flow rate by approx. 1 ton/h

Non nominal steam condition results in a power yield reduction by approx. 6 %

The efficiency of the turbine decreases considerably at low load

It is obvious that the turbine measurement is connected with high uncertainty. The equipment is not calibrated sufficiently and the number of measuring points is also insufficient. Therefore, the major conclusions are based on a qualitative evaluation with few quantitative calculations. For a more accurate performance evaluation it is necessary with a controlled measurement serie with calibrated instruments. One conclusion, however, that needs no investigation is that high load operation is highly desirable.

Future monitoring system

When a thorough performance test has been carried out and the measurement instrumentation has been calibrated, it is possible to develop a monitoring system that - on-line or off-line - monitores the performance of the steam turbine. Based on the results, a numerical model will be derived that transforms the non-nominal results to a nominal basis and use this for comparison between real behaviour and expected behaviour.

12.3 Performance monitoring HNO_3.

In the beginning of the chapter (12.1) it was discussed that performance degradation could be very important when considering large energy conversion (f.x. in a gas turbine). The nitric acid plant is basically build as an advanced combined cycle plant with an almost balancing power shaft. At design values Nitric Acid Plant IV yields 3.6 MW shaft power. The two turbines, however, yield a total of 18.2 MW and the compressors thus use 14.6 MW. Since a considerable part of the profit of producing nitric acid comes from energy production, it is clearly important that the turbo machinery is in top shape. Major stress will therefore be laid on the turbo machinery.

During the last couple of years a significant effort has been done in collecting process data via a spreadsheet. From the process data it is thus the wish to be able to calculate the current efficiency of the equipment.

Under the assumption of ideal gas the isentropic efficiency of the turbo compressors can be expessed as

$$\eta_{is} = \frac{T_{in}\left(\left(\frac{P_{out}}{P_{in}}\right)^{\frac{\gamma-1}{\gamma}}\right)}{T_{out} - T_{in}} \qquad (12.3.1)$$

The accuracy of the model is not very important as long as it shows relative performance under normal operation range. The model can be tuned, using process data for a specified period. This is done for the air compressor in Nitric Acid Plant IV. The isentropic efficiency is calculated using γ=1.4 over a period from November 93 to July 94. The resulting curve is shown in Figure 12.2.

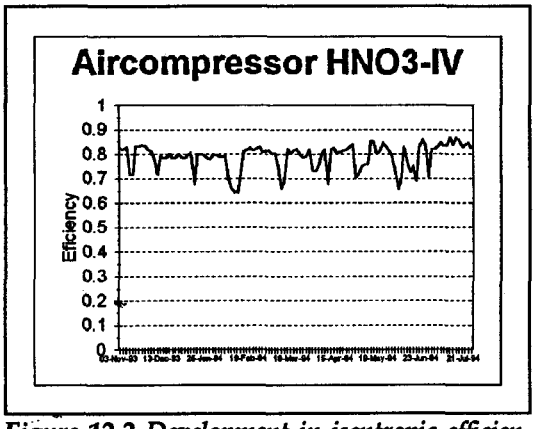


Figure 12.2 Development in isentropic efficiency of air compressor HNO_3 IV.

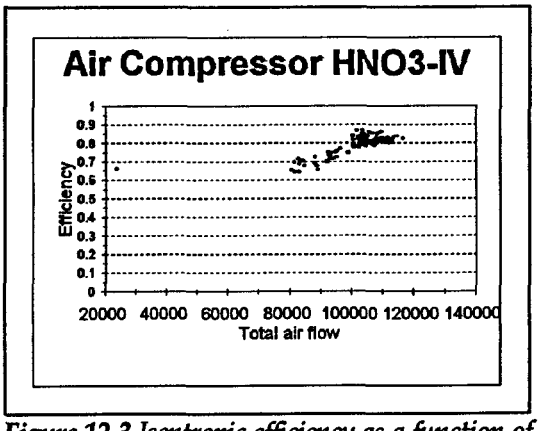


Figure 12.3 Isentropic efficiency as a function of inlet flow rate.

The curve shows the development in isentropic efficiency over time. The information that can be derived from the curve, however, is of limited value, since it does not give any picture of performance characteristic. Next step is to consider the flow rate (nm^3/h) to the compressor. Instead of showing the efficiency versus time it is shown against inlet flow rate (Figure 12.3).

The curve shows that there is a connection between inlet flow rate and isentropic efficiency. The points on the curve are, however, still scattered. To obtain a more precise picture of the performance it is necessary to look at the volumetric flow to rate the compressor instead of normalised flow as obtained from the process data. If ideal gas behaviour is assumed, the corrected flow can be calculated as proportional to the inlet temperature. In figure 12.4 the curve is redrawn using corrected flow. There is now a clear picture of the performance with regard to the corrected flow. It is possible to enhance the model even further by including f.x. air humidity but with all other uncertainties the current model seems to be reasonably accurate.

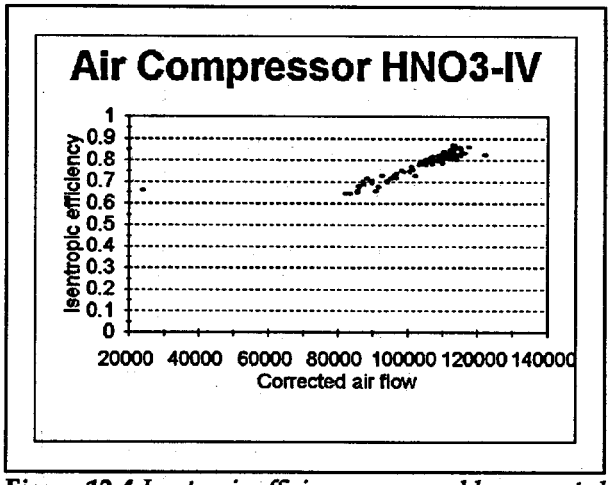


Figure 12.4 Isentropic efficiency expressed by corrected flow.

The curve showed in Figure 12.4 can now act like a reference curve for future performance evaluation. Every operation condition can be placed in the diagram and the distance between expected performance (expressed by isentropic efficiency) and real performance can be evaluated. Distance between expected behaviour and real behaviour can be followed in time and can be used as guideline for deciding when the compressor should be cleaned and/or be taken out for inspection. An outline of the performance monitoring curve is shown in Figure 12.5 where the distance between actual performance and expected performance is shown.

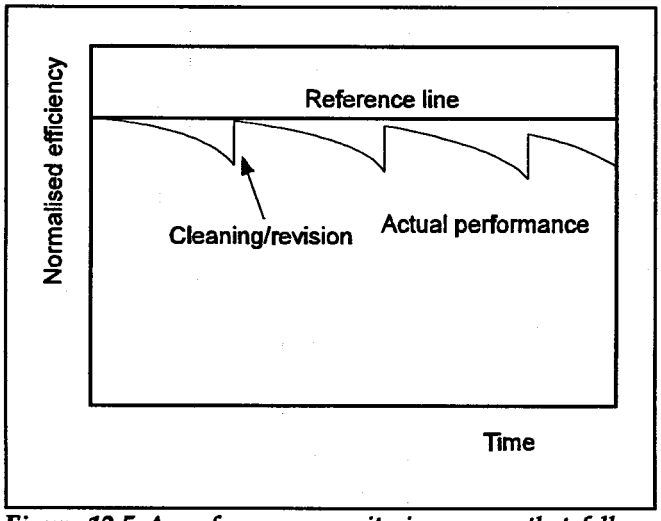


Figure 12.5 A performance monitoring curve, that follows the distance between real performance and expected performance.

A performance monitoring system as outlined here has the advantage of being simple. It can easily be incooperated in the existing data acquisition system (spreadsheet) taking advantage of the buildt-in graphic functions.

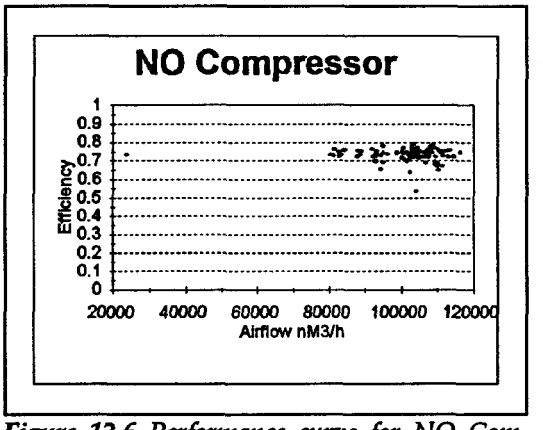


Figure 12.6 Performance curve for NO Compressor.

Similar models can be derived for the NO Compressor and the Tail Gas Turbine, while the assumption of ideal gas is to crude for the steam turbine. There are currently not enough data available for monitoring the Tail Gas Turbine and the Steam Turbine. For the NO compressor the isentropic efficiency seems to be independent of the inlet flowratee (Figure 12.6)[1]. There are however some scatter which can be caused by fluctuations in the amount of NO gas that reacts to NO_2 in the compressor. Further the compressor is water injected with various amount of water. The interpretation of the curve should therefore be done with care. The reference curve is, despite of this, of reasonable value, since it is possible to detect severe degradation using this simple method.

12.4 Performance monitoring - conclusion.

The performance test and monitoring discussed in this chapter have been in simple character. There is, however, no doubt that performance monitoring is an important aspect of process engineering. In this chapter it is shown that large deviation can occur and that it is possible with simple models to construct a monitoring system that reveals severe performance degradation. If the intention is to detect minor divergences it is, however, necessary with more elaborate models and with more accurate measurement instrumentation. This is the case if the operating costs are of special importance. An example of a process where this could be the case is the newly designed Gas Turbine Plant. Here the total economy (operation and depreciation) rely on steady operation efficiency.

[1] This illustrates the inherent difference between the different types of compressors. The air compressor is an axial compressor (high full load efficiency) and the NO compressor is a centrifugal compressor (flat, and lower, efficiency curve).

13
SITE UTILITY OPTIMISATION

This chapter demonstrates how a simple LP formulation of the total utility system (steam mains, gas and steam turbines etc.) can be used for optimisation. The proposed model simulates the marginal performance for all equipment and takes practical constraints into consideration. The model is implemented in a spreadsheet (Excel), where a standard optimiser is used for optimisation.

13.1 Utility system description.

The total utility system is outlined in Figure 13.1. High pressure steam is produced in the sulphuric acid plant, the nitric acid plants and in a boiler. In the near future a new gas turbine is taken into operation with an associated heat recovery boiler.

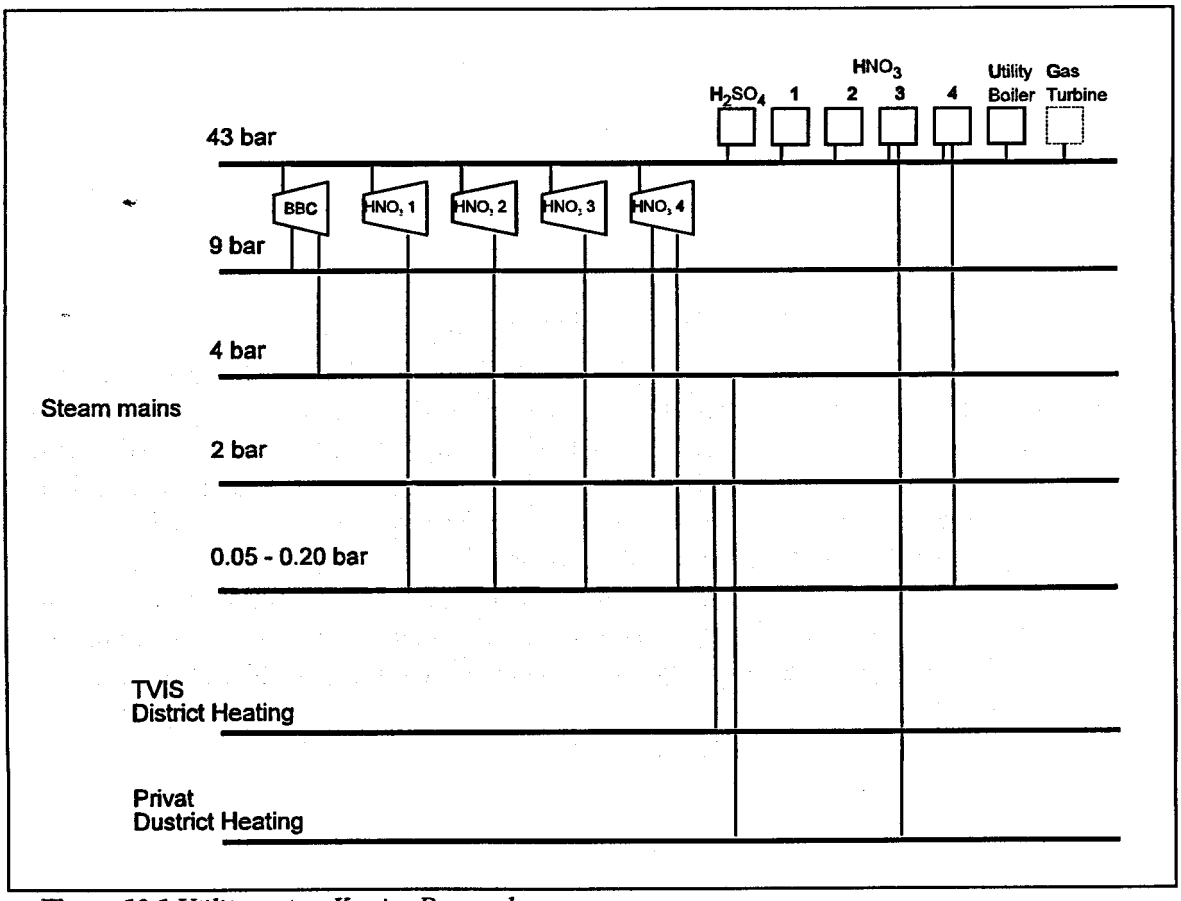


Figure 13.1 Utility system Kemira Danmark.

In this study it is assumed that the steam mains pressures are kept constant at design levels (44 bar, 9 bar, and 4 bar). This assumption seems to be reasonable in accordan-

ce with the actual situation at Kemira. However, as discussed in chapter 13, some disturbances in steam condition can occur. Further in chapter 13 the performance of the BBC steam turbine was discussed. In the present chapter the steam turbines will initially be assumed having design performance.

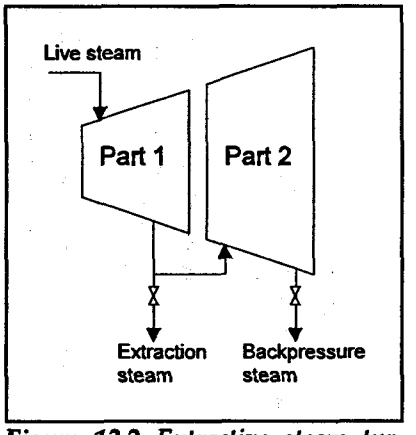


Figure 13.2 Extractive steam turbines are split in two part turbines. Flows are controlled by valves.

From a conceptual view point the extractive steam turbines (BBC and HNO_3) can each be treated in two parts (Figure 13.2). Each part will typically have a flow and pressure ratio specific efficiency η_{is} = f(Steam flow rate, pressure ratio). The pressure ratio can be expressed in terms of an assumed turbine constant (C_t).

$$C_t = \dot{m}_{Steam} \sqrt{\frac{p_1 v_1}{p_1^2 - p_2^2}} \qquad (13.1)$$

where m is the steam mass flow rate, p_1 is the inlet pressure, p_2 is the exit pressure and v_1 is the specific steam volume for the inlet flow.

This expression models the flow rate through the steam turbine. If the pressures are fixed then the flow rate is determined by the above equation. In practice, the extraction pressure will always be higher than the pressure of the associated steam main. To control the extraction flow rate a valve is used. From the above expression it obvious that the lower the load the higher discharge pressure and thus more throttling. This relation obviously results in losses in efficiency. Therefore, maximum efficiency is obtained for full capacity. In the subsequent part a simple rating of the turbine performance will be used, based on the performance map from the equipment suppliers. The rating is based on marginal power production per steam flow rate for each turbine part.

For an extraction steam turbine the following expression is derived

$$Power = C_1 \dot{m}_1 + C_2 \dot{m}_2 - C3 \qquad (13.2)$$

where C_1 and C_2 represent the marginal power production and C_3 is a constant part.

For the new gas turbine system the power production can be calculated as a function of the steam generation at the heat recovery boiler. The natural gas consumption can similarly be calculated as function of steam production.

$$Power = C_1 \dot{m} \tag{13.3}$$

$$Gas\ consumption = C_2 \dot{m} \tag{13.4}$$

13.2 LP formulation of the utility system problem.

With the above performance characteristics for the power production equipment a general LP formulation will be derived for the total utility system.

The objective is to serve the steam users in the most economic way, taking into consideration electricity costs, gas costs and equipment availability. The resulting LP formulation is

$$\text{Max} \quad C_{Tot} = C_E + C_{DH} - C_{Gas} \tag{13.5}$$

s.t

Cost expressions	C_E	$= P_{Tot}\, c_E$
	C_{DH}	$= Q_{DH}\, c_{DH}$
	C_{Gas}	$= V_{gas}\, c_{gas}$
Energy balances	P_{Tot}	$= P_{GT} + P_{HNO3} + P_{BBC}$
	P_{GT}	$= C_{GT,p}\, F_{GT}$
	P_{HNO3}	$= C_{HNO3,L}\, F_{HNO3,L} + C_{HNO3,C}\, F_{HNO3,C} - P_{HNO3,0}$
	P_{BBC}	$= C_{BBC,L}\, F_{BBC,L} + C_{BBC,B}\, F_{BBC,B} - P_{BBC,0}$
	Q_{DH}	$= H\, F_{HNO3,E}$
	F_B	$= V_{B,gas}\, C_B$
	$V_{Gt,gas}$	$= C_{GT,gas}\, F_{GT}$
Mass balances	F_{HP}	$= F_{HNO3,s} + F_{H2SO4} + F_{GT} + F_B$
	F_{HP}	$= F_{HNO3,L} + F_{BBC,L} + F_{th,1} + F_{th,2}$
	F_{MP}	$= F_{BBC,E} + F_{th,1}$
	F_{MP}	$= F_{Proc,MP}$
	F_{LP}	$= F_{BBC,B} + F_{th,2}$
	F_{LP}	$= F_{Proc,LP} + F_{LP,HNO3}$
	$F_{BBC,L}$	$= F_{BBC,E} + F_{BBC,B}$
	$F_{HNO3,L}$	$= F_{HNO3,C} + F_{HNO3,E} - F_{LP,HNO3}$
	V_{gas}	$= V_{GT,gas} + V_{B,gas}$

where

C_{Tot}	Total energy related income	(DKK/h)
C_E	Electricity income	(DKK/h)
C_{DH}	District heating income	(DKK/h)
C_{Gas}	Natural gas expenditure	(DKK/h)
c_E	Specific electricity cost	(DKK/kWh)
c_{DH}	Specific district heating cost	(DKK/GCal)
c_{gas}	Specific natural gas costs	(DKK/Nm^3)
P_{Tot}	Total power production	(kW)
P_{GT}	Gas turbine power production	(kW)
P_{HNO3}	Nitric acid IV power production	(kW)

P_{BBC}	BBC turbine power production	(kW)
Q_{DH}	District heating	(GCal/h)
V_{gas}	Gas usage	(Nm^3/h)
F_{HP}	HP steam main flow	(t/h)
F_{MP}	MP steam main flow	(t/h)
F_{LP}	LP steam main	(t/h)
$F_{Proc,MP}$	Process MP usages	(t/h)
$F_{Proc,LP}$	Process LP usages	(t/h)
F_{H2SO4}	H_2SO_4 steam production	(t/h)
$F_{HNO3,s}$	HNO_3 steam production	(t/h)
F_{GT}	Gas turbine steam production	(t/h)
F_B	Boiler/after burner steam prod.	(t/h)
$F_{BBC,L}$	BBC HP live steam usages	(t/h)
$F_{HNO3,L}$	HNO_3 HP live steam usages	(t/h)
$F_{th,1}$	Throttling HP to MP steam	(t/h)
$F_{th,2}$	Throttling HP to LP steam	(t/h)
$F_{HNO3,E}$	HNO_3 steam extraction (Distr. Heat)	(t/h)
$F_{BBC,E}$	BBC steam extraction (MP)	(t/h)
$F_{HNO3,C}$	HNO_3 - steam to condenser	(t/h)
$F_{BBC,B}$	BBC - Back pressure steam (LP)	(t/h)
$F_{LP,HNO3}$	LP steam to HNO_3 LP section	(t/h)
$C_{GT,2}$	Marginal GT power production	(477 kW/(t/h))
$C_{HNO3,L}$	Marginal HNO_3 part 1 power prod.	(153.5 kW/(t/h))
$C_{HNO3,C}$	Marginal HNO_3 part 2 power prod.	(96.5 kW/(t/h))
$C_{GT,gas}$	Marginal gas usages	(167.1 kW/(t/h))
$C_{BBC,L}$	Marginal BBC part 1 power prod.	(47 kW/(t/h))
$C_{BBC,B}$	Marginal BBC part 2 power prod.	(90 kW/(t/h))
$P_{HNO3,0}$	Power production at no steam flow	(5150 kW)
$P_{BBC,0}$	Power production at no steam flow	(625 kW)
H	Heating value of HNO_3 extr. steam	(0.527 Gcal/t)

Numbers in brackets () are based on design data.

Further inequality constraints are imposed for all variables (0<Var<max). This keeps the equipment within its capacity limit. The proposed model is implemented in a spreadsheet (Appendix A7).

13.3 Using the LP model for daily energy planning.

The proposed model calculates the optimal operation of utility system for a given demand and given energy costs. This is demonstrated with the following conditions

Electricity costs	c_E	=	0.52	DKK/kWh	
District heating value	c_{DH}	=	25	DKK/Gcal	
Natural gas costs	c_{gas}	=	0.75	DKK/Nm^3	
Steam production HNO_3	$F_{HNO3,s}$	=	40	t/h	
MP steam use	$F_{Proc,MP}$ =	6	t/h		
LP steam use	$F_{Proc,LP}$	=	30	t/h	
Max H_2SO_4 steam production	F_{H2SO4}	<	10	t/h	
Max LP steam to HNO_3 turbine	$F_{LP,HNO3}$ <	5	t/h		

The optimal operation point under these conditions is

C_{Tot}	6187	DKK/h
P_{Tot}	17559	kW
P_{GT}	7394	kW (Full load)
P_{HNO3}	5850	kW (Full load)
P_{BBC}	4315	kW (Full load)
Q_{DH}	2	Gcal/h
V_{gas}	4070	Nm^3/h
F_{GT}	15.5	t/h (Constrained)
F_B	18.5	t/h
$F_{BBC,L}$	40	t/h (Constrained)
$F_{HNO3,L}$ 44	t/h (Constrained)	
$F_{th,1}$	0	t/h
$F_{th,2}$	0	t/h
$F_{HNO3,E}$	4	t/h
$F_{BBC,E}$	6	t/h
$F_{BBC,B}$	34	t/h
$F_{HNO3,C}$ 44	t/h (Constrained)	
$F_{LP,HNO3}$ 4	t/h	

Further the marginal cost of process steam is calculated

MP steam marginal cost	53.75	DKK/t
LP steam marginal cost 6.95	DKK/t	

At these conditions with high electricity costs, it is optimal to utilise all power production capacity. With a connection between the 4 bar steam main and the HNO_3 steam turbine/District heating system it is possible to utilise all power producing capacity. The optimisation has also been carried out using lower electricity costs. The results are given in appendix A7.

13.4 LP steam to the HNO_3 turbine system.

In the above LP formulation it has been assumed that it is possible to use LP steam (4 bar) in the second part of the HNO_3 turbine. This connection is not available today. The LP model can be used to evaluate the value of such a connection, under different operation modes. Two scenarios are selected

	Scenario A	Scenario B
LP steam usage	10	20
MP steam usages	3	5

HNO_3 Steam production	35	40

Both scenarios are evaluated under the following conditions

Electricity costs : 0.14, 0.35, 0.52 DKK/kWh
District heating costs : 25, 150 DKK/GCal

The results are given in appendix A7. In Table 13.2 and 13.3 the economic effect is extracted for the two scenarios.

Table 13.2 Scenario A Value of BBC-HNO3 connection DKK/h	0.14 DKK/kWh	0.35 DKK/kWh	0.52 DKK/kWh
25 DKK/GCal	0	192.1	738.6
150 DKK/GCal	0	854.8	1766.1

Table 13.3 Scenario B Value of BBC-HNO3 connection DKK/h	0.14 DKK/kWh	0.35 DKK/kWh	0.52 DKK/kWh
25 DKK/GCal	0	0	296.8
150 DKK/GCal	0	384.3	967.8

There seems to be a large spectrum of situations where LP steam could be used successfully in the HNO_3 turbine low pressure part. Up to 1766 DKK/h could be saved if this option was available. Further preliminary investigations indicate that the marginal efficiency of the BBC turbine at low load is considerably higher than the values used here. This would increase the benefit of using LP steam in the HNO_3 turbine. This is, however, not investigated further here.

If the average saving is in the vicinity of 300 DKK/h then a yearly saving of 2.1 MDKK is possible based on operation 7000 h/yr. This does, however, have to be evaluated in more detail. The investment is considered to be reasonably low (200,000 - 500,000 DKK). All in all the pay back time should be remarkably low for this change.

It is also possible with this model, to evaluate the effect of replacing the existing BBC turbine with a new more efficient turbine.

13.5 Summary and discussion.

In this chapter A simple LP model was applied for the total utility system problem. With this simple formulation it is possible to determine optimal operation point based on the varying energy prices. Further the model can be used for setting internal steam costs that corresponds to the overall costs. This should form a better basis for subsequent process optimisation.

The current models for turbine performance are based on original performance map. It should be noted that these maps are associated with large uncertainties. Therefore when better performance data are obtained these values should be used in the LP formulation. At that stage it could be necessary to use non-linear model to get an accurate performance map.

Finally the option of using LP steam in the HNO_3 IV turbine was evaluated. This shows a potential saving of about 2 M.Dkk/yr with a very reasonable pay back period. It will further give more flexibility in steam distribution, since the BBC turbine will be more independent of the steam users.

14
POWER GENERATION IN THE NPK SECTOR

The major natural gas consumer at Kemira is the NPK sector where the NPK fertiliser product is manufactured (Process description in appendix 4). The gas is used in the spherodizers, where the fertiliser product is formed and dried.

A single spherodizer is fed with an air flow of 60,000 Nm^3/h (21.5 kg/s) heated by natural gas combustion until 300 °C. This results in a considerable exergy loss. The average gas usage in NPK I (8000 h/year) is 1120 Nm^3/h (airflow 57 kg/s).

The aim of this chapter is to exploit the exergy loss in the spherodizer combustor. It is important, however, to take into account the control demand for the process. A modified process must be just as operable and controllable as the existing process. Therefore only proven technology will be used.

14.1 Gas turbine system for the spherodizers.

The exergy loss in the process is mainly caused by the irreversibilities in the natural gas combustion. This exergy loss can be reduced if the combustion takes place at a higher temperature. The heat can thereafter be used in a heat engine. The obvious option is to use a gas turbine, which can operate at temperatures up to approximately 1200 °C.

Efficient gas turbines are only manufactured by a limited number of producers with a limited number of different turbines. It is therefore important to keep in mind that optimisation of the gas turbine system is very constrained.

Two general systems will be evaluated here. In the first system (System A) a gas turbine set will be used with additional air to keep the spherodizer inlet temperature at 300 °C. In the second system (system B) the turbine exhaust gas will be cooled in a steam boiler down to 300 °C. The two systems are outlined in Figure 14.1.

There is still a considerable exergy loss in system A due to the irreversible mixing of cold air (ca. 20 °C) with hot gas turbine exhaust temperature (ca. 500 °C). In system B the exergy loss will be depending of the temperature difference through the boiler, but in general the exergy loss in B will be considerable lower than in case A.

There are, however, other considerations, that must be taken into account. The capital investment for system B must be expected to be higher than for system A. A maybe more important issue is the controllability of the two systems. It is very important that the inlet temperature to the spherodizer can be varied fast in order to maintain high product quality. In the existing process this is controlled by the amount of natural gas fired in the combustor. In system A the temperature can be controlled by the amount of cold air mixed with the exhaust gas. This is, however, not as fast as

the existing system. System B, suffer even more, since changing temperature require a change in steam flow conditions, which might be infeasible or in best case very slow.

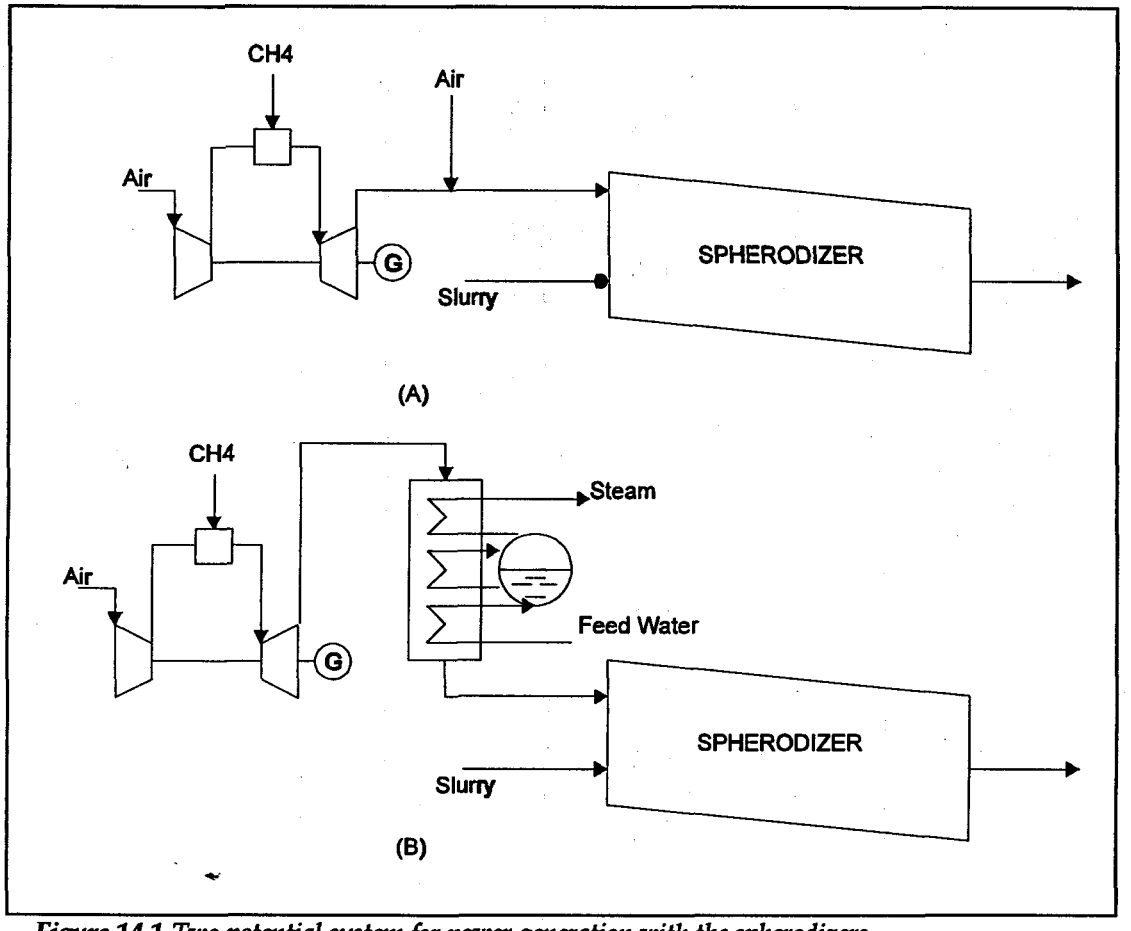


Figure 14.1 Two potential system for power generation with the spherodizers.

It was stated initially that the new process should be just as controllable as the existing. It is thus necessary to add a little more complexity to the systems. In order to avoid down time for the spherodizers it is necessary to maintain the original burners and air supply system. This also has other advantages. It will make it possible to adjust the inlet temperature just as fast as with the original process. When the temperature is too high additional air is supplied with no or very little natural gas combustion, while for too low temperatures the original burners will operate with low air flow rate and high natural gas combustion. Further it is desirable to be able to bypass the spherodizers in case of emergencies. Therefore a by-pass stream with a fast closing valve is included in both systems. The enhanced system lay outs are shown in Figure 14.2 and 14.3.

It was initially mentioned that there is only a limited number of gas turbine candidates for this specific process. To be a candidate the gas turbine must have an exhaust flow rate that matches the spherodizer need. Candidates will be listed for both systems.

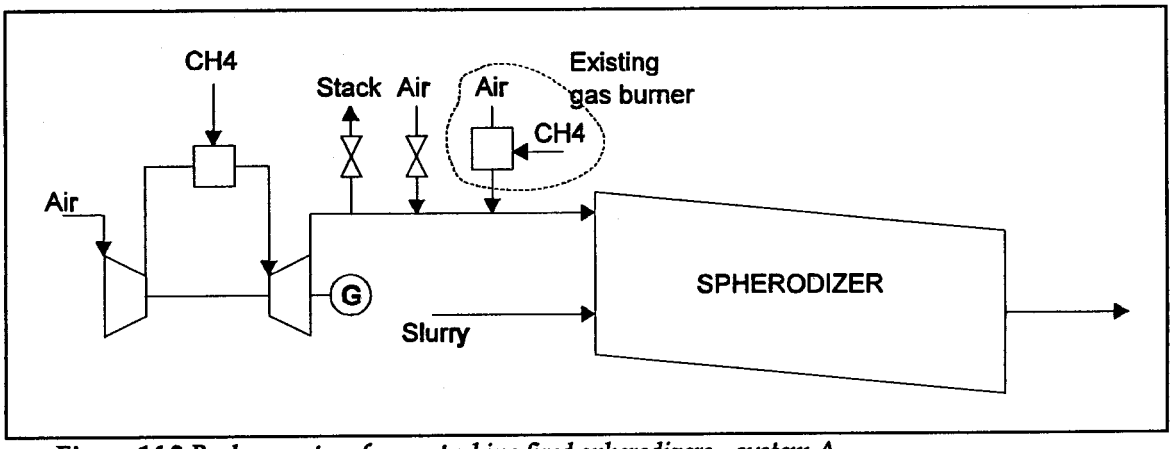


Figure 14.2 Backup system for gas turbine fired spherodizers - system A.

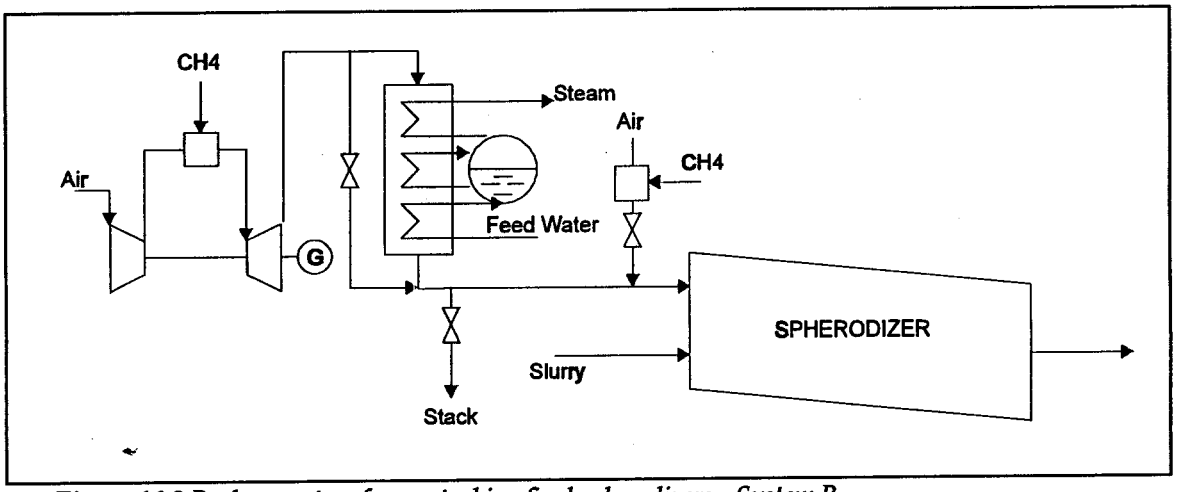


Figure 14.3 Backup system for gas turbine fired spherodizers - System B.

The average hot air (300°C) demand was in 1993 57 kg/s. In the following 50 kg/s will be used as design point (988 Nm^3/h gas consumption).

14.2 System A evaluation.

System A is easily evaluated for all available gas turbine systems listed in table 14.1. The amount of additional air is calculated as the difference between gas turbine exhaust gas flow rate and nominal flow to the spherodizer (50 kg/s). The amount of natural gas fired in the existing burner is determined by the resulting temperature of mixing the exhaust air with the secondary air (this will not happen physically). The values are given in table 14.2.

$$\dot{m}_{sph} = \frac{\dot{m}_{exh} T_{exh} + \dot{m}_{air} T_{air}}{T_{sph}}$$

where m is mass flow rate, T is temperature. Index sph : spherodizer requirement, air : fresh air, exh : gas turbine exhaust. In table 14.2 selected gas turbines candidates are listed.

Table 14.1 Type/Manufacturer	Pressure ratio -	Inlet Temperature °C	Exhaust Temperature °C	Air flow kg/s	Power kW	Estimated cost 10^6 DKK[1]
Alison 501KB7	13.4	1077	536	20.0	4942	15.6
Alison 571KA	12.7	1166	538	19.4	5590	18.2
Dres. Rand DC990	12.5	1049	480	19.4	4200	13.0
Ruston TB5000	7.0	899	488	20.8	3830	11.1
Ruston Tornado	12.0	999	475	27.8	6219	18.9
Solar Taurus	11.2	1016	497	20.6	4370	12.4

Table 14.2 Type/Manufacturer	Power kW	Additional air kg/s	Additional gas firing (Nm^3/h gas)	Total gas usage (Nm^3/h)
Alison 501KB7	4942	30	335	1884
Alison 571KA	5590	30.6	359	1947
Dres. Rand DC990	4200	30.6	462	1783
Ruston TB5000	3830	29.2	388	1759
Ruston Tornado	6219	22.2	123	2008
Solar Taurus	4370	29.4	380	1804

The major capital costs are the gas turbine purchase, Piping and control equipment. While Gas Turbine costs differ among each other the piping and other costs will be assumed fixed.

Piping, foundation	2000	10^3 DKK
Control equipment	1000	10^3 DKK
Engineering	1000	10^3 DKK
Misc.	1000	10^3 DKK

14.3 System B evaluation.

The gas turbine candidates for system B are listed in table 14.3.

[1] 1 US$=6.5 DKK

Table 14.3 Type/Manu-facturer	Pressure ratio -	Inlet Tem-perature °C	Exhaust Temperature °C	Air flow kg/s	Power kW	Estimated cost 10^6 DKK
GE LM1600	21.7	1227	487	44.7	13430	44.9
Mitsub. MF111A	12.8	1135	543	48.1	12826	37.7
NvPgn PGT10	14.0	1068	463	40.3	9980	33.8
Solar Mars	15.7	1057	466	38.1	8840	28.5
Solar Mars	15.7	1104	491	38.3	10000	29.9

System B features some additional degrees of freedom compared with system A. Steam can be raised at various conditions. However, since the potential steam production is limited, it will not be economical feasible to include a new steam turbine. The steam production must therefore be led to a steam turbine with available capacity. This constrains our search to the existing HP steam main, which is at 43 bar and 425 °C.

With this constraint each gas turbine candidate can be evaluated in terms of power output and additional natural gas usage. It is assumed that the feed water is 90 °C and that the marginal power production of the raised steam is approximately 860 kW/(kg/s) steam. The calculated power output etc. are given in Table 14.4. It should be noted that the resulting temperature difference in the boiler is rather high (small heat exchanger area).

Table 14.4 Type/Manufact-urer	Steam production ton/h	Estimated boiler cost 10^6 DKK	Steam Power kW	Gas consump-tion Nm^3/h	Total power output kW
GE LM1600	11.9	10.9	2843	3420	16273
Mitsub. MF111A	16.7	11.3	3989	3810	16815
NvPgn PGT10	9.3	10.5	2222	2792	12772
Solar Mars	9.0	10.2	2150	2584	11424
Solar Mars	10.4	10.0	2484	2815	12815

Other costs are assumed to be the same as for system A:

Piping, foundation	2000	10^3 DKK
Control equipment	1000	10^3 DKK
Engineering	1000	10^3 DKK
Misc.	1000	10^3 DKK

14.4 Project economics.

There are many uncertainties involved in the economics of the project. The major items in the cost evaluation are the average electricity cost, natural gas cost and capital costs. Further it is important to predict the annual down time for the spherodizers. These values can be changing over time due to market changes, political interventions etc.

For evaluation of the system the following values are used

Electricity price	$0.30 + 0.10$[2]	DKK/kWh
Natural gas	0.75	DKK/Nm^3
On line time	8000	h/year
Effective interest	10	%

Table 14.5 System A Type/Manufacturer	Power kW	Additional gas consumption Nm^3/h	Investment 10^6 DKK	Net operational income DKK	Pay back year	NPV (4 years) 10^6 DKK
Alison 501KB7	4942	896	20.6	10.4	2.0	12.4
Alison 571KA	5590	959	23.2	12.1	1.9	15.2
Dres. Rand DC990	4200	795	18.0	8.7	2.1	9.6
Ruston TB5000	3830	771	16.1	7.6	2.1	8.0
Ruston Tornado	6219	1020	23.9	13.8	1.7	19.8
Solar Taurus	4370	816	17.4	9.1	1.9	11.4

Table 14.6 System B Type/Manufacturer	Power kW	Additional gas consumption Nm^3/h	Investment 10^6 DKK	Net operational income DKK	Pay back year	NPV (4 years) 10^6 DKK
GE LM1600	16273	2537	60.8	36.9	1.6	56.2
Mitsub. MF111A	16815	2860	54.0	36.6	1.5	62.0
NvPgn PGT10	12772	1996	49.3	28.9	1.7	42.3
Solar Mars	11424	1831	43.7	25.6	1.7	37.4
Solar Mars	12815	1727	44.9	30.6	1.5	52.1

[2] As a part of the Danish CO_2 tax act, decentralized combined heat and power production is supported. For CHP based on natural gas an award of 0.10 DKK/kWh is given.

14.5 NPK sector - Discussion.

The above preliminary evaluation shows that there is a considerable potential for power production associated with the NPK sector. The marginal power is produced with up to 58% thermal efficiency (GE LM1600). The associated economics looks very favourable.

With the proposed lay-out (Figures 14.2 and 14.3) flexible operation should be secured with the gas turbine integrated systems. There might, however, be some additional costs regarding control system that are not included in this preliminary evaluation.

This evaluation of gas turbine integration in the NPK sector shows some interesting aspects on practical process system engineering. Comparing with the *Synthesis Life Cycle* proposed in chapter 1.3 this study has remained at a low level of detail. With regard to gas turbine selection, however, this has been done at a rather detailed level. This is because the gas turbine selection plays a very dominant role in the synthesis and that this element is one of the most constrained part. Another approach could be to assume fixed gas turbine efficiency and then optimise the gas turbine system and then at a later stage select an appropriate gas turbine. Selection at that stage might show that the assumed efficiencies were wrong and that the optimisation must be redone. This aspect reinforces the need of practical reasoning at every stage of the synthesis.

15
CONCLUSION

This work has aimed at practical synthesis of industrial process plants. All parts of the synthesis have been viewed relative to the *Process Synthesis Cycle* (Chapter 1). Based on a review of existing design approaches different aspects of the overall synthesis are presented in form of a general synthesis procedure for processing system (Chapter 7). As part of the energy synthesis a new framework for industrial heat exchanger network is studied (Chapter 6). This framework is implemented in the *HEN Explorer* software tool. All elements have been used in synthesis of a new nitric acid process (Chapter 10 and Nielsen and Hansen, 1995) and for power production (Chapter 9).

Kemiras major energy consumers have been evaluated for possible energy improvements. While major potential for energy improvements is present, there presently are only few economically feasible improvements. The most promising improvement is integration of a gas turbine system in the fertiliser (NPK) section.

In the following the major achievements in each area of investigation will be outlined.

15.1 Energy synthesis of total processes.

In this work process synthesis and subsequently energy synthesis has been viewed from an abstract point of view focusing on different design technologies' advantages and limitations (Nielsen et al. 1994). A Process Synthesis Cycle has been proposed that illustrates how problems are solved, when levels of information and knowledge are steadily increasing during the work (Chapter 1.3). The process Synthesis Cycle model illustrates how conceptual design and detailed optimisation are interconnected. Practical problems are often initially ill defined. This understanding should be reflected in the initial approaches, which emphasise the conceptual level. Based on an initial synthesis at a conceptual level, a more detailed formulation can be made and additional data included. It is recommended to take a step back after each iteration, checking assumptions etc. and then reformulate the problem. This precaution should reduce the risks that initial assumptions or simplifications preclude competitive alternatives.

An important obstacle for wide use of process synthesis methods is the limited software accessibility. While process simulators are used on a limited scale among the larger industries, dedicated synthesis tools are almost unknown by industry. Pinch technology has for years offered the most successful design methods. The relative high industrial impact is due to the simplicity of the Pinch based approach. However, utilisation of recent development in Pinch Analysis will also require advanced software.

An alternative route has been proposed for general energy synthesis of process plants, based on a standard process simulator with limited pinch analysis capabilities. In the proposed approach the synthesis is started from the initial design by choosing an initial conceptual design. The proposed conceptual design is simulated with the process simulator. All heating and cooling requirements are served by external utilities. The heat exchanger network can thus be represented by the process composite curves. The energy targeting capability can then be used to determine the actual heat and cooling demands for a given process configuration and a minimum approach temperature. For pure exothermic processes, as those mainly treated in this thesis, targeting is done reversed. Here the heating demand is set to zero. Targeting thus gives the resulting minimum approach temperature. A minimum approach temperature less than zero indicates that no feasible heat exchanger network exists for the proposed process. The process can then be optimised in an iterative procedure, where product yield and/or power production can be optimised subject to a minimum allowable approach temperature. The number of important process variables can vary. To reduce the dimension of the resulting problem it is important to utilise additional information and heuristics. This approach is demonstrated in the synthesis of the Humid Air Turbine power cycle, where a multidimensional problem successfully was reduced to a two dimensional problem. This reduction was obtained using heuristics based on the second law of thermodynamics.

The proposed synthesis approach is also tested on synthesis of the sulphuric and nitric acid processes with success. In all cases the approaches are tailored to the specific problem using second law heuristics.

15.2 Improved HEN synthesis.

A new framework for HEN synthesis has been proposed based on a conceptual description of the network elements. While major efforts in HEN synthesis have been directed towards simplified problems the proposed approach allows for more rigorous problem formulation. An object oriented framework is formulated that can be applied at different level of detail in a coherent way. A major advantage of the proposed framework is that it is extendible. It is thus possible within the same framework to include simple auxiliary units, such as pumps, compressors etc.

The proposed framework is implemented in the synthesis tool - *HEN Explorer*. The developed tool is able to handle grassroot design as well as retrofit design. The tool can handle temperature dependent physical properties and detailed heat exchanger specification. Further it allows for specific allocation of exchanger types and price functions for specific matches.

The capability of *HEN Explorer* is tested for a range of literature problems. In most cases *HEN Explorer* has been able to find the better solutions. Especially when handling complicated trade offs as those met in retrofit problems *HEN Explorer* seems superior. This advantage is primarily due to the underlying optimisation algorithm. *HEN Explorer* uses a simulated annealing algorithm that simultaneously asses all variables. It is therefore unique for handling hidden trade offs, while it may require comparatively long computation time.

15.3 Improved process designs.

Routes to improved energy efficiency for two of the world most important chemical processes have been proposed. The improvements require no changes in the core processes. The remaining development work for industrial implementation to full scale is thus limited. Both proposed processes are based on standard equipment.

A new energy integrated nitric acid process for enhanced power production is proposed. With the new integration scheme the specific power production can be raised from approximately 130 kWh/t(HNO_3) to more than 300 kWh/t(HNO_3). Equally important the new process is even simpler than the conventional process since no steam system is required. This simplicity results in a proposed design that is more energy efficient at no additional cost.

The new energy integrated process is based on saturation of the tail gas leaving the absorption column. The result of this modification is an increase in mass flow rate to the tail gas turbine. The new process is optimised using the proposed strategy for energy synthesis as outlined in chapter 7.

A similar enhancement is investigated for the sulphuric acid process. Until now, the atmospheric process has been regarded as the most energy efficient process, while the pressure process is preferable for maximum conversion and reduction in equipment sizes. The analyses in this study prove that maximum conversion and energy efficiency do not necessarily counteract each other. The pressure contact process can thus be optimised to give a superior efficiency (322 kWh/t(H_2SO_4)) compared with the optimised atmospheric process (292 kWh/t (H_2SO_4)).

With saturation of the tail gas in the pressure contact sulphuric acid process it is possible to produce sulphuric acid with a power production up to 356 kWh/t(H_2SO_4). This can be compared with the values for the conventional processes that produces 264 kWh/t(H_2SO_4).

An interesting new aspect of compressor integration has been discovered during the study of the sulphuric acid plant. It has been demonstrated that integrated compressors can be interpreted as heat pumps during the synthesis. Integrated process compressors should thus be treated as conventional heat pumps during the synthesis according to the pinch principles.

15.4 Overall energy improvement at Kemira.

Analyses of the acid processes show that only limited energy reduction can economically be expected. This is mainly due to the high starting cost for any alternation. A detailed study on integrating the principles of the improved nitric acid process in unit IV was conducted. This showed that the existing process, within technical limits, can enhance power production by 30% (1.2 MW worth approximately 2.8 MDKK/yr). Constraints within the existing heat exchanger network, however, cause the cost of necessary changes to be very high. A more simple integration study was conducted where minimum changes to the existing

design were maintained. This case resulted in a more modest improvement (170 kW - 300 kW).

Evaluation of the NPK process shows that there is a considerable potential for power production associated with the NPK sector. The marginal power is produced with up to 58% thermal efficiency (GE LM1600). The associated economics looks very favourable with pay back periods down to two years. With the proposed layout flexible operation should be secured with a gas turbine integrated systems. There might, however, be some additional costs regarding control system that are not included in the preliminary evaluation.

This evaluation of gas turbine integration in the NPK sector shows some interesting aspects on practical process system engineering. Comparing with the *Synthesis Life Cycle* proposed in chapter 1.3 this study has remained at low detailed level. With regard to gas turbine selection, however, this has been done at a rather detailed level. This is because the gas turbine selection plays a very dominant role in the synthesis and that this element is one of the most constraint parts. Another approach could be to assume fixed gas turbine efficiency and then optimise the gas turbine system and then at a later stage select an appropriate gas turbine. Selection at that stage might show that the assumed efficiencies were wrong and that the optimisation must be redone. This reinforces the need of practical reasoning at every stage of the synthesis.

Finally a simple LP model has been applied for the total utility system problem. With this simple formulation it is possible to determine optimal operation points, based on current energy prices. Further the model can be used for setting internal steam costs that correspond to the overall costs. This should form a better basis for subsequent process optimisation. The option of using 4 bar steam from the BBC turbine in the HNO_3 IV turbine was evaluated. This shows a potential saving of about 2 M.Dkk/yr with a very reasonable pay back period. It will further give more flexibility in steam distribution, since the BBC turbine will be more independent of the steam users.

16
REFERENCES

Ackley D.H., G.E. Hinton and T.J Sejnowski, A Learning Algorithm for Boltzmann Machines, *Cognitive Science*, **9**, 147 (1985).

Aarts E.H.L and P.J.M van Laarhoven, Statistical cooling: a general approach to combinatorial optimization problems. *Philips J. Res.* **40**, 193 (1985).

Aarts E.H.L. and P.J.M. van Laarhoven, *Simulated Annealing: Theory and Applications*, New York (1987).

Ahmad S., Heat Exchanger Networks: Cost Trade-Offs in Energy and Capital, *Ph.D. Thesis*, UMIST, Manchester UK, (1985).

Ahmad S and E. Petela, Supertarget: Applications Software for Oil Refinery Retrofit, Paper presented at AIChE Annual Meeting, Houston, March/April (1987)

Ahmad S., B. Linnhoff and R. Smith; Cost Optimum Heat Exchanger Networks-2. Targets and Design for Detailed Capital Cost Models, *Comput. chem. Engng*, **14** p. 751 (1990).

Alefeld G., Probleme mit der Exergie, *BWK* Bd. 40 Nr. 3 (1988)

Amarger R.J., L.T. Biegler and I.E. Grossmann, An Automated Modelling and Reformulation System for Design Optimization, *Computers chem. Engng* **16** p. 623 (1992).

Andrecovich M.J. and A.W. Westerberg, A single synthesis method on utility bonding for heat integrated distilation sequences, AIChE J., **Vol. 31**, 363, 1985.

Árvá P., B. Csukás, Computer-aided process synthesis by fuzzy valuated structures. *Computers chem. Engng* **12**, p. 215 (1988).

Biegler L.T., On the simultaneous solution and optimization of large scale engineering systems. *Computers chem. Engng*, **12**, p. 357 (1988).

Boehm R.F. (Editor), Thermodynamics and the design, analysis, and improvements of energy systems, ASME Winter Annual Meeting, Anahaim November (1992).

Calandranis J. and G. Stephanopoulos, A Structural Approach to the Design of Control Systems in Heat Exchanger Networks. *Comput. chem. Engng* **12**, p. 651 (1988).

Cameron G.M., P.D. Nolan and K.R. Shaw, Pressure contact Process, *Chem. Eng. Prog.*, **74** p. 47 (1978).

Cerda J., A.W. Westerberg, D. Mason and B. Linnhoff. Minimum Utility Usage in Heat Exchanger Network Synthesis - a transportation problem. *Chem. Engng. sci.* **38**, 373 (1983).

Cerdá J. and M.R. Galli, Synthesis of Flexible Heat Exchanger Networks-II.Nonconvex Networks with Large Temperature Variations. *Comput. chem. Engng* **14**, p. 213 (1990b).

Cerdá J., M.R. Galli, N. Camussi and M.A. Isla, Synthesis of Flexible Heat Exchanger Networks-I. Convex Networks. *Comput. chem. Engng* **14**, p. 197 (1990a).

Ciric A.R., C.A. Floudas, A Retrofit Approach for Heat Exchanger Networks. *Computers chem. Engng* **13**, p. 703 (1989).

Ciric A.R and C.A Floudas, A Mixed Integer Nonlinear Programming Model for Retrofitting Heat Exchanger Networks, *Ind. Eng. Chem. Res.* **29** p. 239 (1990).

Coldberg R.D., M. Morari and D.W. Townsend, A Resilience Target for Heat Exchanger Network Synthesis. *Comput. chem. Engng* **13**, p. 821 (1989).

Das H., P.T. Cummings and M.D Le Van, Scheduling of serial multiproduct batch processes via simulated annealing. *Computers chem. Engng* **14**, 1351 (1990).

Dhole V.R, Distillation column integration and overall design of subambient plants, PhD Thesis, UMIST, Manchester, 1991.

Dhole V.R. and B. Linnhoff; Setting Targets for Distilation, Part 1, *Process Engineering*, June p.33 (1992).

Dhole V.R. and B. Linnhoff; Setting Targets for Distilation, Part 2, *Process Engineering*, July p.37 (1992).

Dhole V.R. and B. Linnhoff; Setting Targets for Distilation, Part 3, *Process Engineering*, August p.39 (1992).

Dhole V.R., B. Linnhoff; Total site for fuel, co-generation, emmisions, and cooling. Computers chem. Engng, Vol. 17 Suppl, pp S101-S109 (1993).

Dhole V.R., B. Linnhoff; Overall Design of Low Temperature Processes, *Comput. chem. Engng*, **18**(Suppl.), p. S105 (1994).

Dhole V.R. and B. Linnhoff; Distillation Column Targets, *Comput. chem. Engng*, **17**, p. 549 (1993).

Dolan W.B, P.T. Cummings and M.D Le Van, Process Optimisation via Simulated Annealing: Application to Network Design. *AIChE Jl* **35**, p. 725 (1989).

Dolan W.B, P.T. Cummings and M.D Le Van, Algorithmic Efficiency of Simulated Annealing for Heat Exchanger Network Design. *Comput. chem. Engng* **14**, p. 1039 (1990).

Douglas J. M., *Conceptual Design of Processes*, McGraw-Hill, Inc., New York (1988).

El-Sayed Y.M., Targeting an Optimal Design of Heat Exchange in Power System. *Thermodynamics and the Design, Analysis, and Improvement of Energy Systems*, ASME AES Vol. 27, New York (1992).

Floudas C.A, A.R. Ciric and I.E. Grossmann, Automatic Synthesis of Optimum Heat Exchanger Network Configurations. *AIChE Jl.*, **32**, p. 276 (1986).

Floudas C.A., A.R. Ciric, Strategies for Overcomming Uncertainties in Heat Exchanger Network Synthesis. *Computers chem. Engng* **13**, p. 1117 (1989)

François M. and K. Boris, SYNEP1 : a methodology for energy integration and optimal network synthesis. *Computers chem. Engng* **13**, 603 (1989).

Gaggioli R.A. and P.J. Petit, Use the second law first. *Chem Tech*, 496 (1977).

Gaggioli R.A., D.A. Sama, S. Qian and Y.M. El-Sayed; Integration of a New Process Into an Existing Site - A Case Study in the Application of Exergy Analysis, *ASME Journal of Engineering for Gas Turbines and Power*, **113**, 170 (1991).

Galli M.R. and J. Cerdá, Synthesis of Flexible Heat Exchanger Networks-III. Temperature and Flowrate Variations. *Comput. chem. Engng* **15**, p. 7 (1991).

Geman S., Geman D., Stochastic relaxation, Gibbs distributions and the Bayesian restoration of images. *IEEE Trans. Patt. Analysis Mach. Intell.* **6**, 721 (1984).

Grossmann I.E. and R.W.H. Sargent, Optimum Design of Chemical Plants with Uncertain Parameters, *AIChE J.*, **24**, p. 1021, (1978).

Grossmann I.E., Mathematical Methods for Heat Exchanger Network Synthesis, *IEA Workshop on Process Integration - International Experiences and Future Opportunities*, Göteborg, Sweden (1992).

Gundersen T and L. Ness, The Synthesis of Cost Optimal Heat Exchanger Network Synthesis - An Industrial Review of the State of the Art, *Comput. chem. Engng.* **12**, p.503 (1988).

Gundersen T. and I.E. Grossmann, Improved Optimization Strategies for Automated Heat Exchanger Network Synthesis through Physical Insight. *Comp. and Chem. Engng.* **14**, (1990).

Gundersen T, Achievements and Future Challenges in Industrial Design Applications of Process System Engineering. *4th International Symposium on Process System Engineering*, Quebec, Canada August (1991).

Hall S.G., Targeting for Multiple Utilities in Pinch Technology, *Ph.D. Thesis*, UMIST, Manchester UK, (1989).

Hall S.G., S. Ahmad, R. Smith; Capital cost targets for heat exchanger networks comprising mixed materials of construction, pressure ratings and exchanger types, Computers chem. Engng, Vol 14, No. 3, pp 319-335, 1990.

Hall S.G., S.J. Parker and B. Linnhoff; Process Integration of Utility Systems, Paper presented at the IEA Workshop on Process Integration, Gotenburg, (1992).

Hansen M.W and J.S. Nielsen, Energy Optimisation of a Nitric Acid Plant - An Introduction to Pinch Technology (In danish), dk-TEKNIK, (1991).

Harvey S.P., K.F. Knoche and H.J. Richter, Improvement of Gas Turbine Power Plant Efficiency through Off-Gas Recycling. *ASME Winter Annual Meeting, Anaheim 1992*, AES-Vol27 (1992).

Hohmann, E.C., *Optimum Networks for Heat Exchange*, Ph.D. Thesis, Univ. So. Calif. (1971).

Jezowski J, SYNHEN: Microcomputer Directed Package of Programs for Heat Exchanger Network Synthesis. *Comput. chem. Engng* **16**, p. 691 (1992).

Jones D.A., A.N. Yilmaz and B.E. Tilton, Synthesis Techniques for Retrofitting Heat Exchanger Networks, *Chem. Engng. Prog.*, **82** p. 28 (1986).

Kalina A.I, H.M Leibowitz D.W Markus and R.I. Pelletier, Further Technical Aspects and Economics of a Utility-Size Kalina Bottoming Cycle, *ASME Paper No.91-GT-365*, (1991).

King G, *Seperation Processes*, McGraw-Hill, New York, (1971).

Kirkpatrick S.C, C. Gelatt and M. Vecchi, Optimisation by simulated anneaking, *Science* **220**, p. 671 (1983).

Kolas T.J., The exergy Method of Thermal Plant Analysis, Butterworth, London (1985).

Laarhoven P.J.M. van and E.H.L. Aarts, *Simulated Annealing: Theory and Applications*, D. Reidel, Dordrecht (1987).

Linnhoff B. and J.R. Flower, Synthesis of Heat Exchanger Networks: I Systematic Generation of Energy Optimal Networks, *AIChE Jl* **4**, p. 633 (1978a).

Linnhoff B. and J.R. Flower, Synthesis of Heat Exchanger Networks: II Evolutionary Generation of Networks with Various Criteria of Optimality, *AIChE Jl* **4**, p. 642 (1978b).

Linnhoff B. and J.R. Flower, A Thermodynamic Approach to Practical Process Network Design, Paper presented at AIChE Annual Meeting, San Francisco, Nov. (1979).

Linnhoff B. et al., User Guide on Process Integration for the Efficient Use of Energy. Institution of Chemical Engineers, London (1982).

Linnhoff B., New concepts in thermodynamics for better chemical process design. *Chem. Eng. Res. Des*, **61**, 207 (1983).

Linnhoff B. and D.R. Vredeveld, Pinch Technology has Come of Age, *Chem Eng Prog*, p. 33, July (1984).

Linnhoff B. and S. Ahmad, Supertargeting: Optimal Synthesis of Energy Management Systems, *ASME Winter Annual Meeting*, Anaheim, Dec. (1986).

Linnhoff B. and S. Ahmad, Supertargeting: Optimal Synthesis of Energy Management Systems, *Trans ASME, Journal of Energy Resources Technology*, **111**, p.131. (1989).

Linnhoff B., Pinch Technology for the Synthesis of Optimal Heat and Power Systems. *Trans ASME, J of Energy Resources Technol*, **111**, p. 137 (1989).

Linnhoff and S. Ahmad; Cost Optimum Heat Exchanger Networks-1. Minimum Energy and Capital Using Simple Models for Capital Cost, *Comput. chem. Engng*, **14** p. 729 (1990).

Linnhoff B. and F.J. Alanis; Integration of a New Process Into an Existing Site - A Case Study in the Application of Pinch Technology, *ASME Journal of Engineering for Gas Turbines and Power*, **113**, 159 (1991).

Linnhoff B., Pinch analysis and exergy - a comparison. *Energy system and ecology conference*. Cracow, Poland (1993).

Mizsey P, Z. Fonyo, Toward a more realistic overall process synthesis - The combined approach. *Computer chem. Engng*, **14**, 1213 (1990).

Nielsen J.S, Energy optimization by Simulated Annealing, *ASME Winter Annual Meeting, New Orleans*, November (1993).

Nielsen J.S, V. Briones-Vallejo and A.C. Kokossis, An Integrated Framework for the Optimal Design Of Heat Recovery Systems, Paper presented at AIChE annual meeting San Francisco, November (1994)

Nishida N.G., G. Stephanopoulos and A.W. Wetserberg, A Review of Process Synthesis, *AIChE Jl* **27**, p. 321 (1987).

Otten R.M., Layout compiler annealing applied to the floorplan design. *Handbook of Advanced Semiconductor Technology and Computer Systems*. (G. Rabbat, Ed.). Reinhold, New York (1988).

Papoulias S. A. and I. E. Grossmann, A structural optimization approach in process synthesis-I. Utility systems. *Computers chem. Engng* 7, 695 (1983a).

Papoulias S. A. and I. E. Grossmann, A structural optimization approach in process synthesis-II. Heat Recovery Networks. *Computers chem. Engng* 7, 707 (1983b).

Papoulias S. A. and I. E. Grossmann, A structural optimization approach in process synthesis-III. Total processing systems. *Computers chem. Engng* 7, 723 (1983c).

Parker S.J., Supertargeting for Multiple Utilities, *Ph.D. Thesis*, UMIST, Manchester UK, (1989).

Perry R.H., D.W. Green and J.O. Maloney, *Perry's Chemical Engineers' Handbook*, McGraw-Hill, New York (1984).

Press W.H., B.P. Flannery, S.A Teukolsky, W.T. Vetterling, *Numerical recipes in pascal, the art of scientific computing*. Cambridge University Press, Cambridge (1989).

Price D.W., G. Tsatsaronis, Design analysis of Dow-based power plants. *Thermodynamics and teh Design, Analysis, and Improvements of Energy Systems*, ASME AES-Vol. 30, New York (1993).

Polley G.T, M.H.P. Shahi and F.O. Jegede, Pressure drop considerations in the retrofit of heat exchanger networks, Trans IChemE, **68**, p. 212 (1990).

Polley G.T., M.H.P. Shahi and P. Nunez, Rapid Design Algorithms for Shell-and-Tube and Compact Heat Exchangers, Trans IchemE, **69**, 435 (1991a).

Polley G.T and M.H.P. Shahi, Interfacing Heat Exchanger Network Synthesis and Detailed Heat Exchanger Design, Trans IChemE, **69**, p. 445 (1991b).

Rao, A.D., Process for Producing Power, *US Patent 4,829,763* (1989).

Reistad G.M. and R.A. Gaggioli, Available-Energy Costing. ACS Symposium Series, Thermodynamics: Second Law Analysis, No. 122 (1980).

Richter H.J. (Editor), Thermodynamics and the design, analysis, and improvements of energy systems, ASME Winter Annual Meeting, New Orleans November (1993).

Rosen M.A., Assesment of an Integrated Coal-Gasification Combined-Cycle (IGCC) Power Plant Using Energy and Exergy Analyses. *Thermodynamics and the Design, Analysis, and Improvement of Energy Systems*, ASME AES Vol. 27, New York (1992).

Saboo A.K., M. Morari and R.D. Colberg, RESHEX: An Interactiv Sofware Package for the Synthesis and Analysis of Resilient Heat-Exchanger Networks-I. Program Description and Application. *Comput. chem. Engng* **10**, p. 577 (1986).

Saboo A.K., M. Morari and R.D. Colberg, RESHEX: An Interactiv Sofware Package for the Synthesis and Analysis of Resilient Heat-Exchanger Networks-II. Discussion of Area Targeting and Network Synthesis Algorithms. *Comput. chem. Engng* **10**, p. 591 (1986).

Sander U.H.F., H. Fischer, U. Rothe and R. Kola, *Sulphur, Sulphur Dioxide and Sulphuric Acid*, The British Sulphur Corporation Ltd, London (1984).

Shahi M.H.P., Pressure Drop Consideration in Process Integration, Ph.D. Thesis, University of Manchester Institute of Science and Technology, UK (1992).

Shokoya C.G., Retrofit of heat exchanger network for debottlenecking and energy savings, Ph.D. Thesis, University of Manchester Inst. of Sci. and Tech., Manchester (1992).

Smith J.M. and H.C. Van Ness, Introduction to chemical engineering thermodynamics, McGraw-Hill, New York (1987).

Smith R. and B. Linnhoff; The design of separators in the context of overall processes. Chem Eng Res Des, **Vol.** 66, 1988.

Smith R. and P.S. Jones; The optimal design of integrated evaporation systems, Heat Recovery Systems and CHP **Vol 10**, No. 4, p. 341, 1990.

Stecco S.S, U. Desideri, B.Facchini and N. Bettagli, The Humid Air Cycle: Some Thermodynamic Considerations, *ASME Paper No.93-GT-77* (1993).

Stecco S.S, U. Desideri and N. Bettagli, The Humid Air Cycle: A Possible Optimization, *ASME Paper No.93-GT-178* (1993).

Tjoe T.N.; Retrofit of Heat Exchanger Networks, *Ph.D. Thesis*, UMIST, Manchester UK (1985).

Tjoe T.N. and B. Linnhoff; Using Pinch Technology for Process Retrofit, Chem Engng. Journal, **93**, 47 (1986).

Tjoe T.N and B. Linnhoff; Achieving the Best Energy Saving Retrofits, Paper presented at AIChE Annual Meeting, Houston, March/April (1987).

Townsend D.W, B. Linnhoff; Heat and Power Networks in Process Design, Part I: Criteria for Placement of Heat Engines and Heat Pumps in Process Networkss, *AIChE Journal*, **29**, 742 (1983a).

Townsend D.W, B. Linnhoff; Heat and Power Networks in Process Design, Part II: Design Procedure for Equipment Selection and Process Matching, *AIChE Journal*, **29**, 748 (1983b).

Townsend D.W. and B. Linnhoff, Surface area targets for heat exchanger networks, *IChemE 11th Annual Research Meeting on Heat Transfer*, Bath 1984.

Valero A., F.J. Royo, Second Law Efficiency and the Relative Free Energy Function, *Thermodynamics and the Design, Analysis, and Improvements of Energy Systems*, ASME AES-Vol. 27, New York (1992).

von Spakovsky M.R., R.B. Evans, The Optimal Design and Performance of Thermal Systems and Their Components, *Analysis and Design of Advanced Energy Systems: Fundamentals*, ASME AES Vol. 3-1, New York (1987).

von Spakovsky M.R., R.B. Evans, The Design and Performance Optimization of Thermal Systems. *Journal of Engineering for Gas Turbines and Power*, **112**, p. 93 (1990).

Westerberg A.W., A Review of Process Synthesis, in *Computer Applications to Chemical Engineering*. R.G. Squires and G.V. Reklaitis (eds.), ACS Symposium Series. No. 124, Washington (1980).

Westerberg A. W., Synthesis in engineering design. *Computers chem. Engng* **13**, 365 (1989).

Westerberg A.W., An Overview of Process Integration Methodolgies, *IEA Workshop on Process Integration - International Experiences and Future Oportunities*, Göteborg, Sweden (1992).

Woolséy R.E.D. and H.S. Swanson, *Operation Research for Immediate Applications*, Harper and Row, New York (1975).

Woudstra Th., N. Woudstra, Exergy analysis of hot gas cleanup in IGCC systems. *Thermodynamics and the Design, Analysis, and Improvements of Energy Systems*, ASME AES-Vol. 30, New York (1993).

Xiao Y., R. Lin and R. Cai, System Optimization of Humid Air Turbine, *ASME Paper No.94-GT-240* (1994).

Yee T.F. and I.E. Grosmann, Simultanous Optimization Models for Heat Integration - II. Heat Exchanger Network Synthesis. *Comp. and Chem. Engng.* **14**, 1165 (1990).

Yee T.F. and I.E. Grossmann, A screening and Optimization Approach for the Retrofit of Heat-Exchanger Networks, *Ind. Eng. Chem. Res.* **30**, p. 146 (1991).

Zhelev T., Piping Cost Optimization for Heat Exchanger Networks, *The 1994 IChemE Research Event*, London, January (1994).

PAPERS

AES-Vol. 30/HTD-Vol. 266, Thermodynamics and the Design, Analysis,
and Improvement of Energy Systems
ASME 1993

OPTIMIZATION OF ENERGY SYSTEMS BY SIMULATED ANNEALING

Jan Sandvig Nielsen
Kemira Denmark
Vedbæk
Denmark

ABSTRACT

Simulated Annealing is presented as an optimizing method well suited for enhancing energy optimization methods. The basic idea and strategy of the method are presented through examples. A general computer code for implementing the method is given along with a complete code for a simplified problem. Finally the paper gives general guidelines on how to implement simulated annealing in various thermodynamic optimization methods.

INTRODUCTION

Optimizing an engineering system is - generally speaking - a complex task. A high number of continuous and discrete variables are often necessary in order to describe the system in a sufficient way. The mixture of continuous and discrete variables makes it rather difficult - especially for non-mathematicians - to perform a computer-aided optimization of the system. The purpose of this paper is to describe a rather new technique for optimizing such systems. A method that seems to be well suited for a wide range of engineering problems. Though the method is based on somehow complicated mathematics the basic idea and strategy is easily understood and the implementation of the method is almost straightforward.

The method described is called "Simulated Annealing" and has in the last few years achieved much attention. The method has been applied to a wide range of problems including: Design of integrated circuits (Kirkpatrick et al., 1983), Image analysis (Geman and Geman, 1984), Training of neural networks (Ackley et al.,1985), Floor planning (Otten, 1988), Batch-process scheduling (Das et al., 1990) and Design of heat exchanger networks (Dolan et al., 1990). This paper is not intended to be a thorough review of the mathematics involved. Rather it is a short introduction to the main principles of the method.

OPTIMIZATION OBJECTIVES

The central issue in an optimizing assignment is - from a given state - to find a better and if possible an optimum state. As an illustrative example for describing the procedure in Simulated Annealing, we consider a mountainous landscape (Figure 1) where we are standing at a random point. Our task is to find the deepest valley in the area. The most logical way is to head downhill by the rule of steepest descent. If we follow that strategy we will soon find a valley where any immediate adjacent points are at higher elevation. We have found a minimum, but we have no way to be sure that this is the deepest valley in the whole area. There might be a deeper valley on the other side of a mountain range. This indicates that if our goal is to find a global optimum we must allow ourselves temporarily to move uphill in order to get to a deeper valley.

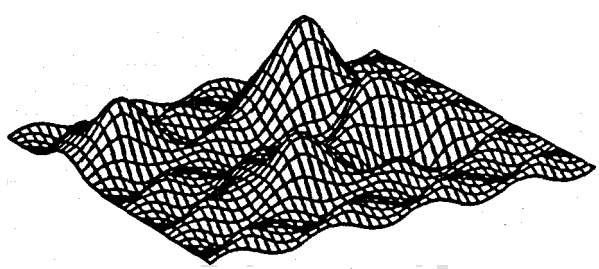


Figure 1. A two dimensional objective function can be viewed as a landscape. The minimum of the objective function is given as the lowest valley in the landscape.

In contrast with most other optimizing strategies Simulated Annealing allows us to move uphill. When we follow the strategy given by Simulated Annealing we will take a step in a random

direction. If the step is downhill we will accept it. If it is uphill we may accept it. The "may" is actually the most important feature in Simulated Annealing. In practice this "may" means that there is a probability **p** that the step is accepted. If the step is downhill the probability **p** is 1. If the step uphill is lifting us **ΔH**, the probability **p** of accepting the step is

$$p = e^{-\frac{\Delta h}{\beta}}$$

The parameter β determines how steep we are allowed to move upwards. With a high value of β the possibility of moving upward is high while a value of β near zero will means that all attempts to move upwards will be rejected. While decreasing the value of β we are able to make a search that initially allows us to move out of local minimums and finally to a global minimum. With a sufficiently high starting value of β and a sufficiently slowly decreasing scheduling, the algorithm will lead us to an optimum or near-optimum state. It has been mathematically proven that the probability of finding an optimal state moves towards unity as the starting value of β and the decreasing schedule moves toward infinity (Laarhoven and Aarts, 1987).

The overall procedure when using Simulated Annealing can be shown in this pseudo-Pascal code:

```
Begin
  Initialize β
  Initialize starting point
  Calculate objective value of starting point
  Repeat
    Repeat
      Make a random step
      Calculate difference in objective function (ΔH)
      If downhill then accept step
      If uphill then "maybe" accept step
                ( prob=exp(ΔH/β))
    until sufficient move
    Decrease β ( β_new = β_old · α)  ( 0 < α < 1)
  Until β is sufficiently small
End.
```

This pseudo code is actually all the optimizing related programming needed. Therefore the main task - when using Simulated Annealing - is to describe the system involved in a way that allows us to make random changes in the system. When the system is well-described we have to experiment to find good values of β and α.

A computer program that optimizes the function $f(x) = x^2(1+\sin(x)/2)$ is given in the appendix. As shown in figure 2, this function has a large number of local minimums. The code, that consists of less than 100 lines, shows the simplicity of the implementation work. When optimizing another function (or set of functions), simply change the objective function and the transition procedure.

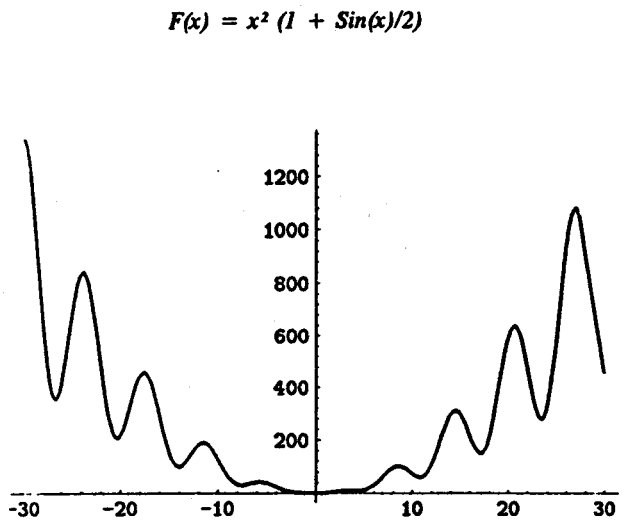


Figure 2. A one dimensional objective function with multiple local minimums. A computer code for optimizing this function is given in the appendix.

When running the code for this example with different optimization parameters (Initial value of β, α) it is noticed that the quality of the solution is dependent of these parameters. If it is important that the solution is a true global optimum, the optimization parameters must be adjusted such that the initial value of β is very high and the decreasing schedule is very slow (α near 1). In most engineering cases, however, the objective function is based on predicted costs whose uncertainties must be considered. Therefore, usually a near optimum solution is sufficient. With the example in figure 2, every solution in the range $-3 < x <$ three is probably equally good.

The implementation work, based on Simulated Annealing, can be split into three parts

Define objective function

Define possible moves

Adjust optimization parameters

Thus the major part of the optimization assignment is to describe the physical behavior of the system and only a little effort is needed for implementation of the optimization routines.

MATHEMATICAL ISSUES

Although we do not want to go deeply into the details, some mathematical insight might be useful when building new applications. When using the Simulated Annealing algorithm, we continuously attempt to transform the current configuration into another configuration in the immediate neighborhood. The

outcome of every attempt is only depending on the previous configuration. This is mathematically known as a Markov Chain. It is important though that the transition algorithm is capable of reaching every possible state in the solution area. One of the main considerations is to allow the transition algorithm to move backwards.

EXAMPLE PROBLEM

The Traveling Salesman Problem (TSP) is an often used example when it comes to global optimization because it belongs to a class of minimization problems for which the objective function has many local minima (Press et al, 1989). In short the Travelling Salesman Problem is to find the shortest route in which a salesman can visit a given number of cities. When following the example problem we first have to define our objective function. In this case we simply want to find the shortest route in which n cities are visited. Therefore, the objective function can be given as

$$\sum_{j=1}^{n}\sqrt{(x_j-x_{j+1})^2-(y_j-y_{j+1})^2}$$

where each city is given by its coordinate (x,y). From the n'th city we return to the starting city $[(x_{n+1},y_{n+1}) = (x_1,y_1)]$. The next step is to define our transition procedure. A simple way to rearrange the route is simply to switch the order of which two cities are visited. With these short descriptions of the objective function and the transition procedure, it is easy to rebuild the computer code for this application. A more efficient set of moves is to remove a section of cities and place the section in another part of the route. A complete computer code using this rearrangement strategy is given by Press et al. (1989).

PINCH BASED OPTIMIZATION

A traditional pinch-based optimization is based on composite and grand composite curves. These are in turn based on the assumption of fixed process streams. In most industrial studies, however, the process streams are not fixed (f.x. Hansen and Nielsen 1991, 92). One example of a non-fixed process stream is heat recovery from a flue gas. In this case we want only to cool down the flue gas as far as the heat can be utilized. In a process plant with multiple non-fixed process streams, the pinch method can be applied in an iterative way.

First an initial guess, for all non-fixed process streams, is applied. Then the total cost of energy and equipment is determined by supertargeting (Linnhoff and Ahmad 1986). Depending on the results from supertargeting, the non-fixed process streams are updated and a new supertargeting is performed. This is done until an optimum state is found for all non-fixed process streams. The updating procedure can be applied using heuristics, linear and nonlinear programming, or other methods. However, the risk of getting caught in a local optimum is high if the number of non-fixed process streams exceeds a few.

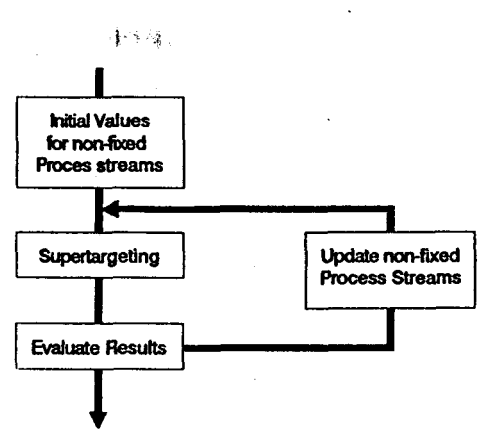


Figure 3. Pinch based iterative optimization in case of multiple non-fixed process streams.

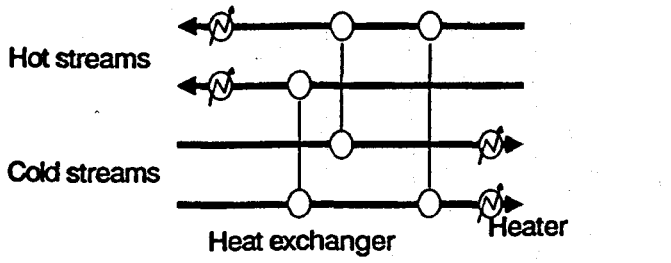
Implementation of simulated annealing in the updating procedure diminishes the risk of getting lost in a local minimum. Again implementation of simulated annealing is almost straightforward and the new targeting procedure is outlined below.

```
(* Global targeting *)
Begin
  Initialize β
  Initial guess of non-fixed process streams
  Calculate total cost of initial guess (Super targeting)
  Repeat
    Repeat
      Make a random change in a random non-fixed
          process stream
      Calculate difference in total cost (ΔCost)
      If difference is < 0 then accept change
      If difference is > 0 then accept change with the
                         probability p=exp(ΔCost/β)
    Until sufficient changes
    Decrease β
  Until β is sufficiently small
End.
```

The targeting procedure is only the first step in a pinch-based energy optimization. The next step is the actual design of the heat exchanger network. The pinch method gives some general guidelines on how to design the network, primarily based on splitting the network in two parts by the pinch (Linnhoff et al. 1982). The total network synthesis can, however, be done without any pinch point and minimum temperature difference assumptions, by applying simulated annealing directly to the problem. Dolan et al. (1990) have applied simulated annealing to the network synthesis problem outlined below.

The objective function in this case is given as the net present value of expenses. It is, in other words, the sum of capital investments and energy costs. The transition procedure proposed by Dolan et al. operate with a range of moves. *Add exchanger* inserts an exchanger between two streams. *Delete exchanger* deletes an exchanger. *Change heat load* changes the amount of

heat exchanged in a random exchanger. *Shift heat load* shifts the heat load of two exchangers. In addition to these moves Dolan et al. operate with stream split where a process stream is split in two part-streams. An interactive program based on this description has been developed and used in several studies (Nielsen 1992, Hansen and Nielsen 1992). The use of the program has led to a dramatic decrease in network design time.



Energy costs : Σ Heat + Cooling supply cost

Capital costs : Σ Heat exchanger investments

Objective value : Net cash flow

Figure 4. Heat exchanger network. The optimization task is to find the heat distribution giving the lowest net present value.

Optimization of non-fixed process streams can also be included in the network synthesis procedure. This is done by applying the extra move *Change non-fixed stream*.

The combination of pinch method and simulated annealing has been used for industrial studies. One example that has been carried out was retrofitting a nitric acid plant at KEMIRA Danmark. The task was optimization of the production of high pressure steam. The overall procedure for the optimization process is outlined in figure 5.

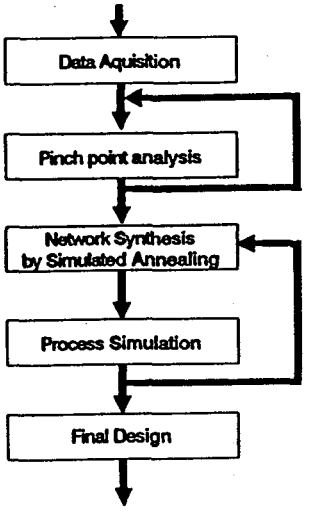


Figure 5. Procedure for retrofitting a nitric acid plant (Hansen and Nielsen 1992).

The changes proposed from the study gave an increase in high pressure steam production of 10 % (60 % increase in steam export) with a pay back period of less than two years.

SECOND LAW BASED OPTIMIZATION

Second law approaches to thermodynamic problems have the obvious advantages of determining the true thermodynamic efficiencies and losses in each process component. One approach to the second law analysis is the one proposed by Sparkovsky and Evans 1990 based on thermoeconomic functional analysis. Here the operating costs are based on the second law quantities that each component requires to perform its function. Component functions relate the entropy generated in each process to the second law quantities that each component exchange with the rest of the system. These functions are set up in a general set of equations that consist of an objective function with multiple constraints. The optimization problem can then be solved by non-linear programming. There is, however, no way to be sure that the results are actually the global optimum due to the nature of nonlinear problems.

A more descriptive thermoeconomic optimization model is the one described by El-Sayed (1989,1992). This model is based on a decomposition of the synthesis problem into a set of modeled basic processes for convenient structural changes (figure 6). The search for optimum decision variables depends on the complexity of the problem. Thus for problems with few design variables a gradient-based method can be used, while for larger problems a judgement-based method is needed. Again the nonlinear nature of the problem can cause failure of standard gradient-based methods.

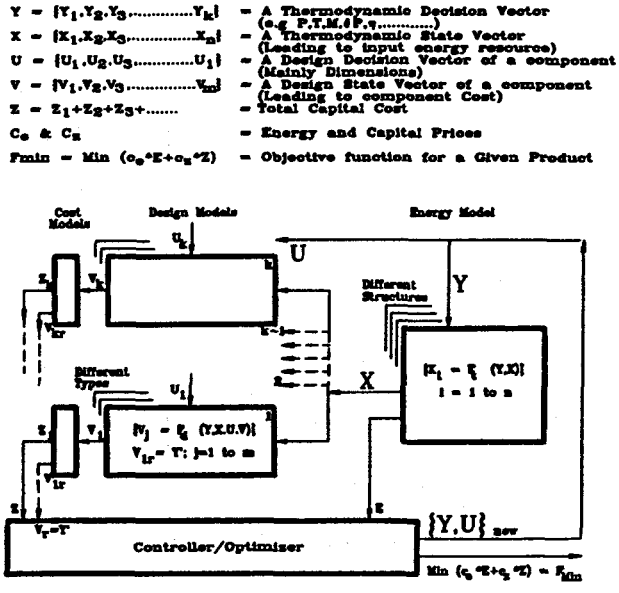


Figure 6. A thermoeconomic optimization framework proposed by El-Sayed (1992).

Both approaches seem to be well suited for implementation of simulated annealing.

CONCLUSIONS

With Simulated Annealing, engineers have another excellent tool for optimizing tasks. One of the primary advantages with Simulated Annealing is the simplicity in the implementation work. With the examples given in this text, most engineers should be able to build their own applications. The major drawback is the computation time. Therefore the method is best suited for problems where the objective function is known to be difficult to optimize either because of discontinuities or because of risks of local minimums.

In energy optimization tasks, where the objective functions in many cases are known to be complex, simulated annealing isan excellent supplement to thermodynamic methods.

ACKNOWLEDGEMENT

Support for this project was provided by Kemira Danmark, dk-TEKNIK - Danish Boiler Owner's Association and the Danish Academy of Technical Science.

NOMENCLATURE

p	=	Probability
ΔH	=	Change in height
x,y	=	Independent variables
α, β	=	Simulated Annealing optimization parameters
ΔCost	=	Change in objective value

REFERENCES

Ackley D.H., G.E. Hinton and T.J Sejnowski, A Learning Algorithm for Boltzmann Machines, *Cognitive Science*, **9**, 147 (1985).

Das H., P.T. Cummings and M.D Le Van, Scheduling of serial multiproduct batch processes via simulated annealing. *Computers chem. Engng* **14**, 1351 (1990).

Dolan W.B., P.T. Cummings and M.D. Le Van, Algorithm efficiency of simulated annealing. *Computers chem. Engng* **14**, 1039 (1990).

El-Sayed Y.M., A Decompostion Strategy for Thermoeconomic Optimization. *Journal of Energy Resources Technology*, **111**, 111 (1989).

El-Sayed Y.M., Targeting an Optimal Design of Heat Exchange in a Power System. *Thermodynamics and the Design, Analysis, and Improvement of Energy Systems*, ASME AES-Vol.228, New York (1992).

Geman S., Geman D., Stochastic relaxation, Gibbs distributions and the Bayesian restoration of images. *IEEE Trans. Patt. Analysis Mach. Intell.* **6**, 721 (1984).

Hansen M.W. and J.S. Nielsen, *Energy analysis of a nitric acid plant* (in Danish), dk-TEKNIK, Copenhagen (1991).

Hansen M.W. and J.S. Nielsen, *Retrofitting a nitric acid plant at Kemira* (in Danish), dk-TEKNIK, Copenhagen (1992).

Kirkpatrick S., C.D. Gelatt and M.P. Vecchi, Optimization by simulated annealing. *Science* **220**, 671 (1983).

Laarhoven P.J.M. van and E.H.L. Aarts, *Simulated Annealing: Theory and Applications*, D. Reidel, Dordrecht (1987).

Linnhoff B. et al., *User Guide on Process Integration for the Efficient Use of Energy*. Inst. Chem. Engrs., UK (1982).

Linnhoff B. and S. Ahmad, Supertargeting: Optimum Synthesis of energy management system. *Computer-Aided Engineering of Energy Systems, Vol. 1 -Optimization.* AES-Vol.2-1, New York (1986).

Nielsen J.S., *Heat exchanger optimization* (in Danish). dk-TEKNIK, Copenhagen (1992).

Otten R.M., Layout compiler annealing applied to the floorplan design. *Handbook of Advanced Semiconductor Technology and Computer Systems*. (G. Rabbat, Ed.). Reinhold, New York (1988).

Press W.H., B.P. Flannery, S.A Teukolsky, W.T. Vetterling, *Numerical recipes in pascal, the art of scientific computing*. Cambridge University Press, Cambridge (1989).

Spakovsky M.R. von, R.B. Evans, The Design and Performance Optimization of Thermal Systems. *ASME Journal of Engg. for Gas Turbines and Power*, **112**, 86 (1990).

Appendix Example of pascal code for optimizing the function Obj(x) = x^2 (1 + Sin(x)/2)

```
Program SaDemo;
const MaxMove = 400;
      MaxSuccess = 100;
      MinimumBeta = 0.0001;
      Alpha = 0.95;
      DeltaX = 3;

var   Beta,Cost,NewCost,X,NewX : real;
      Move, Success, Step      : integer;

Function Objective(X:real):real;
begin
  Objective:=1+Sqr(X)*(1+Sin(X)/2);
end;

Procedure Transition(Var X:real);
begin
  X:=X+DeltaX*(0.5-Random);
end;
```

```
Function AcceptMove(DeltaCost:real):boolean;
begin
  if (DeltaCost < 0) then AcceptMove:=True
  else
  begin
    AcceptMove:=(exp(-DeltaCost/Beta)>Random)
  end
end;
begin
  Randomize;
  Beta := 100000;          {Initialize Beta}
  X    := random*50;       {Starting Point}
  Writeln('Starting Point X = ',X:10:4);
  Cost := Objective(X);
  Step :=0;
  Repeat
    Success:=0;
    Move:=0;
    Repeat
      NewX := X;  {Make Working Copy}
      Transition(NewX);
      NewCost := Objective(NewX);
      if AcceptMove(NewCost-Cost) then
      begin
        X:=NewX;
        Cost:=NewCost;
        Success:=Success+1;
      end;
      Move:=Move+1;
    Until ((Move > MaxMove) or (Success > MaxSucces));
    Beta:=Alpha*Beta;
    Step:=step+1;
  Until Beta < MinimumBeta;
  Writeln('Minimum is ',Cost:8:4,'  Located at ',X:8:4);
  Writeln('After ',Step,' Step');
end.
```

Paper 225g presented at AIChE annual meeting San Francisco November 1994

An Integrated Framework for the Optimal Design of Heat Recovery Systems

J.S Nielsen[1], V. Briones-Vallejo[2] and A.C. Kokossis[2]

Within the last 10 years a large number of publication has aimed at solving the general industrial heat exchanger network problem. Despite of the effort important design issues have not yet been adequately adressed and solved. Furthermore, the existing design technologies, apart from few exceptions, still remain either purely thermodynamic or purely mathematical. The former provide an insightful perspective and are capable of identifying a small number of promising alternatives out of very large and seemingly complex problems. However, their limitations become evident in screening among few but competitive scenarios, as well as in making available systematic procedures for automation. Although employing powerful optimisation techniques and being more rigorous and systematic, the mathematical methods are restricted by the complexity of their design models which even in their simplest versions, give rise to local optima and require extensive tuning of their algorithmic parameters. A possible result of the different design philosophies involved is that no systematic effort has been made so far in order to integrate the existing design techniques and couple their advantages to address the size and complications of industrial applications.

A new approach is presented in this paper which is based upon an integrated analysis of the heat exchanger network problem and is applicable to both synthesis and retrofit designs. As progressing from higher to lower levels of abstraction, the approach employs pinch technology, mathematical programming, and stochastic optimisation in a coordinated fashion that combines the complementary features of each method. At an elevated stage, pinch technology is used in order to develop targets, simplify the problem and accommodate for an insightful perspective. Mathematical programming is used next in order to systematically extract structural information and set up prospective stream matches and networks which are further optimised using a tailored simulated annealing algorithm. The algorithm is capable of exploiting all the design information at this level, and uses an object oriented representation whose architecture accounts for the extendibility of the integrated technology to the general design problem. Its implementation differentiates among different types of streams and heat exchangers, various property models and cost functions, and different design objectives. The potential of the approach is illustrated with two example problems and comparison with other methods.

[1] KEMIRA Danmark, P.O. Box 100, DK-2950 Vedbaek, Denmark

[2] UMIST, Department of Process Integration, P.O. Box 88, Manchester M60 1QD, UK

Design technologies and perspectives

Thermodynamics provide an approach for identifying promising process heat recovery potential. The thermodynamical approach is based on a combination of engineering insights and visualization of the heat transfer between process streams. It is mainly based on identifying the thermodynamical inefficiencies within a given heat exchange system. The most successful use of these principles is the Pinch Technology, which enables the designer to predict the energy and capital targets ahead of design and get guidelines on how to achieve these targets. Since the late 70s pinch technology has been developed by Linnhoff and coworkers at UMIST as a complete methodology, which enables the fundamental understanding of the problem and reduces its combinatorial nature by applying targeting and decomposition. At the time Pinch Technology emerged it was focused on heat exchanger networks. The scope today includes separation system (Smith and Jones 1990, Dhole and Linnhoff 1993), heat and power integration (Linnhoff 1986, Dhole and Zheng 1993) etc. The technology has moved toward a general targeting method and can be applied as a tool for screening and scoping among different process alternatives. The shift toward process analysis and targeting rather than design makes it natural to refer to the method as Pinch Analysis rather than Pinch Technology (Linnhoff 1993). Pinch Analysis is a well tested approach which is able to provide information and guidelines to the designer at a high abstraction level. Although Pinch Analysis is able to screen among several alternative process alternatives it is less efficient when selecting between few competitive alternatives. In other terms, Pinch Analysis is efficient for high level decisions but cumbersome for detailed analysis.

Mathematical methods on the other hand offer a systematic evaluation of detailed alternatives. Mathematical programming approaches have established a methodology which is based upon the development of a reducible system representation inclusive of all possible design scenarios. The representation, known as superstructure or hyperstructure of the problem, is further modeled and optimized using algorithmic techniques. However, because a superstructure (or hyperstructure) is generally comprised by units and streams whose number increase combinatorial with the size of the problem, the mathematical programming approaches face an exponentially increasing computational burden in embracing more structural and operational alternatives. The situation, formally described as a NP-hard problem, imposes limitations on the methodology and the availability of appropriate solvers. The presence of discontinuities and complex nonlinearities makes it difficult to use off-the-shelf optimization procedures. To make the task practicable most methods are based on decomposing the problem into minor problems with the subsequent risk of getting caught in a topology trap.

A special branch of mathematical methods is the stochastic methods. These methods, whos origin should be traced in the analysis and optimisation of clusters, are based on random search methods. They are to some extend insensitive to the discontinuities and complex nonlinearities. They are thus less exposed of getting caught in local optima. The stochastic methods can handle all sorts of complexity and are not dependent on gradients. They are therefore well-suited for combinatorial problems. The positive features of stochastic methods are all of a cost in computational efficiency. With no algorithmic or physical insights the stochastic methods will become costly in terms of computational efforts.

All of the above approaches have produced good solutions on different problems. Each approach seems to have its advantages and limitations. Moreover, there are apparent complementary features among these technologies in terms of potentials and limitations. But

so far no systematic effort has been made for their integration. Instead we have seen that the different approaches have been extended to cover all levels of abstraction. In addition to the lack of integrated analysis to address the problem there are also important industrial aspects that are often disregarded to made the particular technology applicable and/or efficient. Among the frequent assumptions are those of constant heat capacity, countercurrent heat exchange, differentiable cost functions. Gundersen and Grossmann (1990) described the situation: With over 200 publications most of which in the last 8 years "It may come as a surprise that important design issues have not yet been adequately addressed and solved". The surprise reflects on the industrial experience where current practice is based on engineering experience and insight and to some extend on Pinch Analysis. There is only limited use of detailed design methods. This is probably because the problems are oversimplified and because the lack of flexible and efficient tools. What is needed are integrated approaches that better address the industrial problem.

Design integration schemes.

The different design technologies (engineering insights, trageting and mathematical methods) have been discussed and put in perspectives for integration schemes by Kokossis (Kokossis 1993). At the highest level engineering insights is used for a preliminary screening and decomposition with regard to process hierarchy. At an intermediate level targeting methods set goals. Finally at the low level mathematical methods perform detailed optimal designs. These technologies are set in perspective by viewing the approaches as "Design Engines" working between levels of abstraction (Figure 1). Engineering Insight (IE) deliver work with high efficiency at high level. If the approachs is applied at a more detailed level difficulties will arise. The targeting methods (TG) deliver good work at the intermediate level but face difficulties at the high level as well at the low level. Finally Mathematical Methods (MM) deliver work with high efficiency at the low detailed level, while it has difficulties in delivering work at high abstraction level. In the past different schools have tried to extend their methods to cover all levels of abstraction. Figure 1 clearly impose that this is not an efficient use of technologies. What is proposed here is a "combined design engine" that coordinates the effort in a way that give maximum efficiency at each level and allow for full engineering participation. The general approach is perfectly applicable to the heat exchanger network problem, where it is proposed to start with a hierarchical decomposition in order to initialize the problem (deriving process streams). As a next step a targeting methods such as Pinch Analysis is proposed and finally mathematical methods are applied for detailed optimisation (Figure 2). The combined approach utilize the potential of each one of the approaches as well as minimize the limitations.

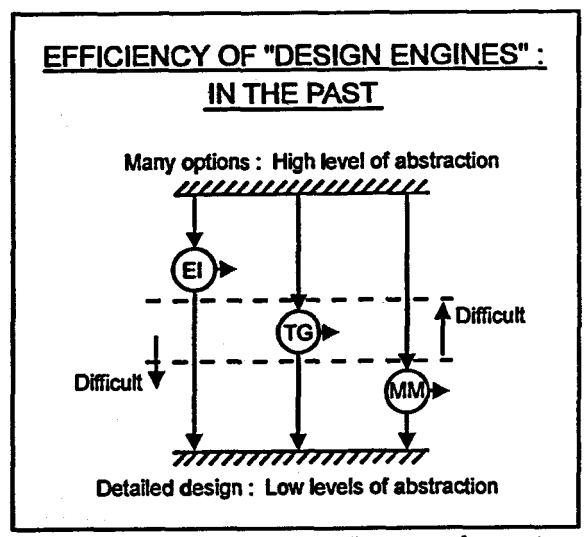


Figure 1 The "Design Engines" versus abstraction.

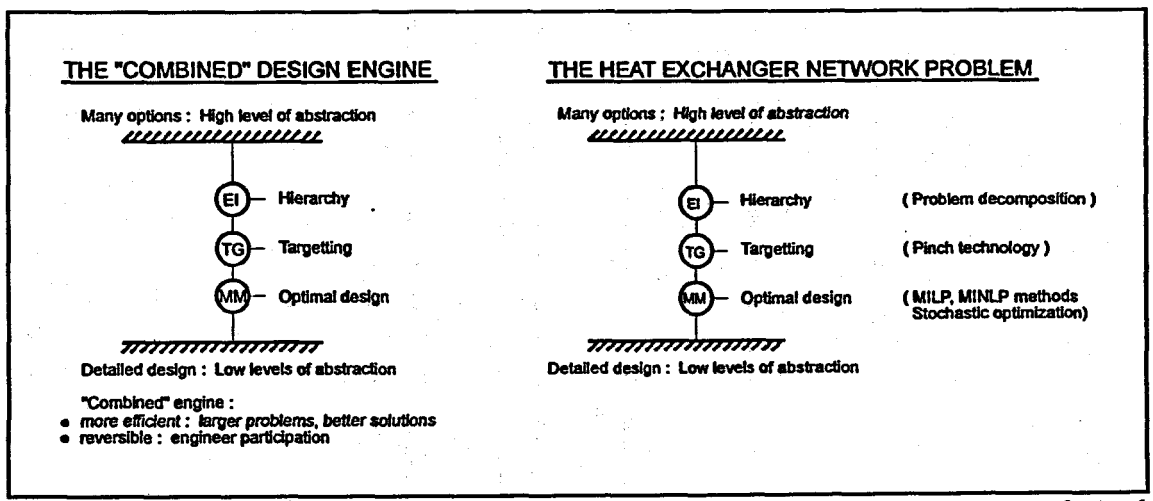


Figure 2 The combined Design Engine. Using technologies at levels where optimum efficiency is obtained.

Technology integration for Heat Exchanger Networks.

The "Combined Engine" approach adds a new perspective to the HEN problem. In order to fully address the general industrial HEN problem it is necessary to readdress the structure of the problem. This require better modelling and efficient network representation. The modelling challenges are to account for different objectives (Grassroot design, Retrofit), streams with variable properties, choices among heat exchanger types etc. The keyword for this is extendability.

The heat exchanger network can be conceptualized in two elements - Streams and Units. With the streams there are associated models for state variables (fx. T-Q relations) and heat transfer variables (fx. heat transfer coefficients h). The units in a heat exchanger network are typically heat exchangers, splits and mixers. Associated with each unit are models for heat transfer, mass balances and energy balances. The two conceptual elements can be represented in two hierarchies - one for streams and one for units (Figure 3).

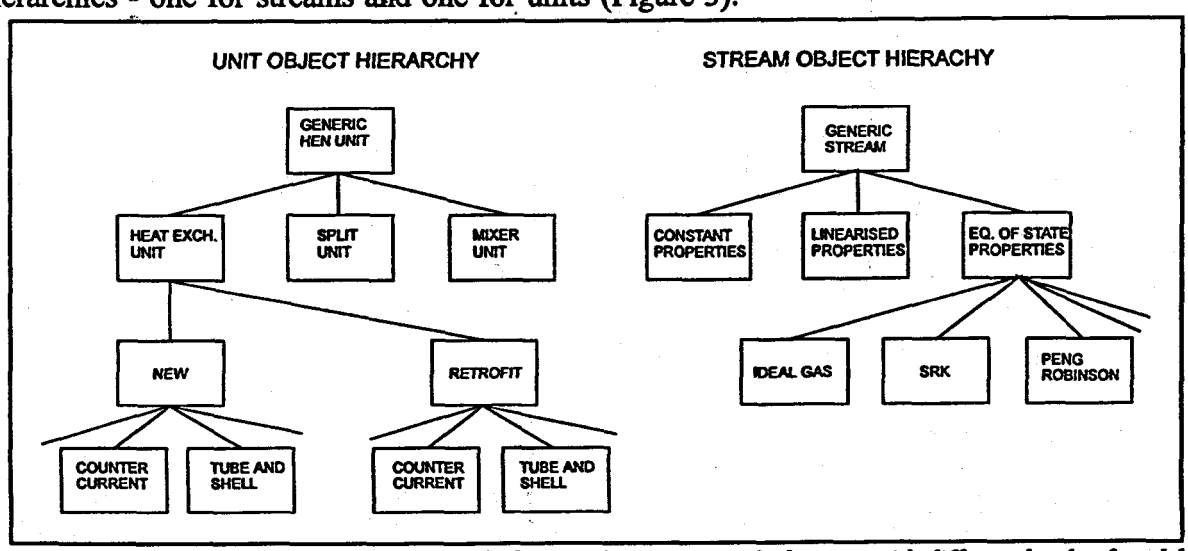


Figure 3 A hierearchical rperesentation of the heat exchanger network elements with different levels of model complexity.

The stream hierarchy has a generic stream object as the ancestor for a range of different stream models. All stream models derived from the generic stream model have models for Q-T relations and h-T relations. The simplest model for a stream is one with temperature independent properties (C_p and h constant). A more detailed model is the linearized model where C_p and h are linearized over a limited number of temperature levels. Finally a full property model can be applied using an equation of state representation.

In the unit hierarchy each object is derived from a generic HEN unit model. Each object derived from the generic HEN object have methods for mass and energy balances, sizing and cost estimation. The three basic unit types are heat exchangers, splits and mixers. For all these basic types there can be distinguished between new units and retrofit units. And at an even lower level a distinguish can be made between heat exchanger types (Counter current, Tube and shell, plate etc.). The proposed representation has several advantages. First of all it is flexible. The same representation can be used to solve the simplified problem (constant properties, countercurrent heat exchange and global price functions) as well as the full industrial problem (advanced property models, complex heat exchangers and match dependent price functions). The representation is easily implemented in an object oriented environment taking advantages of the latest compiler technology. Within an object oriented framework the model can be extended allowing increasingly complex models.

A graphical illustration of the combined approach show that the detail level also vary with the level of abstraction (Figure 4). At high level only limited details are considered while at the lowest level all details are considered. As well as using different method according to abstraction level it is suggested to use appropriate model complexity at each abstraction level.

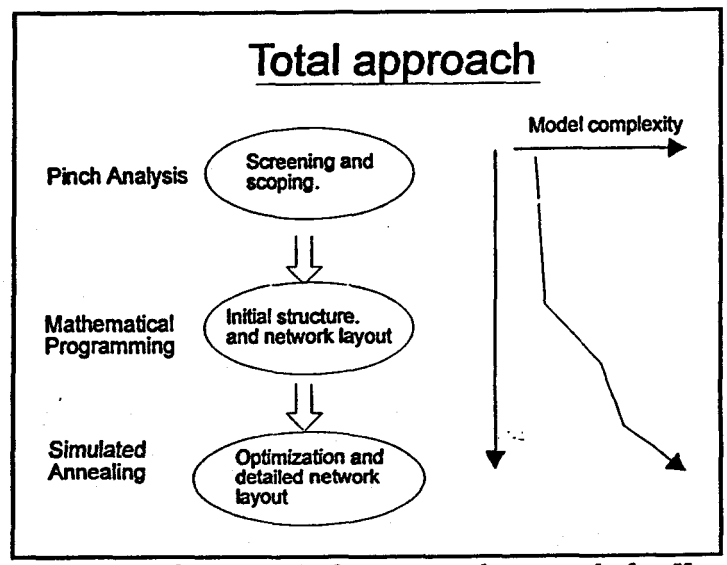


Figure 4 Implementation of a structural approach for Heat Exchanger Network Synthesis with increasing model complexity.

Examples.

The potential of an integrated design along the line proposed is illustrated with two examples. Streams and cost functions of the first example are showed in Table 1. The problem is solved using a tailored Simulated Annealing algorithm. The result of using this approach alone is given in Table 2. The results are averaged over 8 - 10 runs on a 486 PC. The results show that there is a trade off between the quality of solution and computational time.

	T-start K	T-target K	CP kW/K	h kW/m²/K
C1	288.8	650.0	24.795	0.8753
H1	630.6	338.9	7.913	1.6097
H2	583.3	505.6	5.803	0.7265
H3	555.6	319.4	2.374	0.5586
H4	494.4	447.2	31.652	0.7299
H5	477.8	311.1	6.331	0.3541
H6	422.2	383.3	65.943	0.4848
CW	300.0	333.3	-	0.6324

Exchanger cc :	$1300 * Area^{0.6}$	CU/year
Furnace cc :	$321.089 * Q^{0.7}$	CU/year
Fuel cost :	174.022	CU/kW/year
CW cost :	4.634	CU/kW/year

Table 1 Processstream and cost functions for example 1.

Computational time	Average optimum	Standard deviation
100	760000	32000
200	710000	14000
400	685000	8000
800	651000	3500
1600	647000	2400
5000	645500	1450

Table 2 Stand alone result using a Simulated Annealing algorithm.

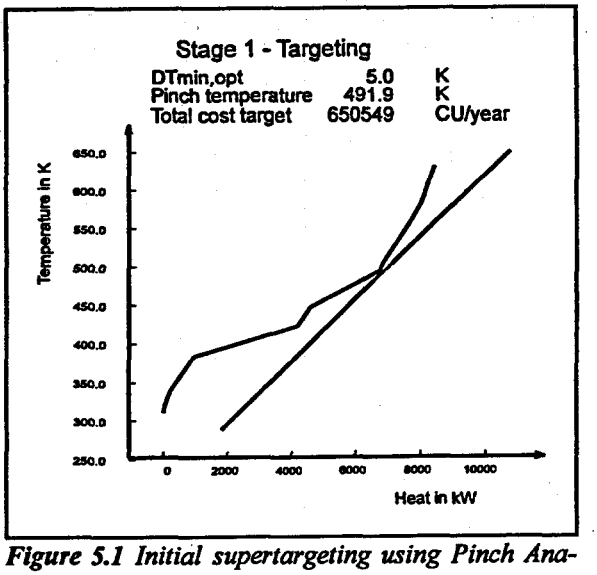


Figure 5.1 Initial supertargeting using Pinch Analysis.

In comparison the combined approach is applied. The approach is illustrated in Figure 5.1 through 5.3. Targeting give an optimum ΔT_{min}= 5 K with a target total cost of 650549 CU/year. With the targeted ΔT_{min} a simple MILP algorithm was applied. This gave an initial network structure that finally was passed to the Simulated Annealing algorithm for detailed optimisation. In the Simulated Annealing algorithm ΔT_{min} and number of units are relaxed. The average result when applying the simulated annealing gave a total network cost of 647128 CU/year within an average computational time of 122 second. When compared with the stand alone approach an order of magnitude improvement in computational time can be observed.

In the case so far counter current heat transfer is assumed. If there instead is applied a tube and shell heat exchanger model it can be seen what effect it has on the result. To determine the number of shells in each match the X_p parameter is used (Ahmad and Smith 1990). This parameter represents the ratio of actual effectiveness to maximum possible effectiveness. A value X_p = 0.9 have been chosen in this example. The maximum size of a single shell is set

to 400 m². With the multipass heat exchanger model three optimization paths has been evaluated.

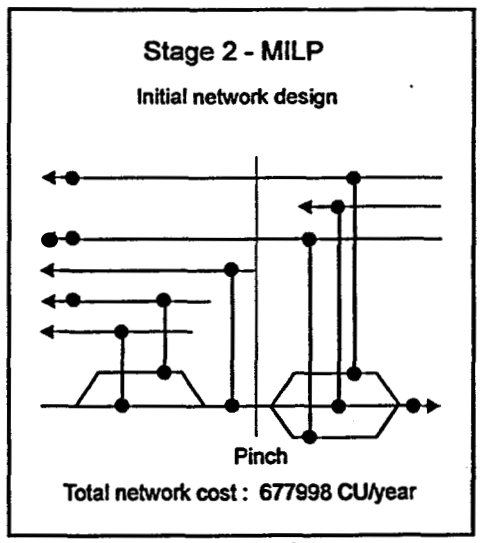


Figure 5.2 Initial network lay out using a simple MILP algorithm.

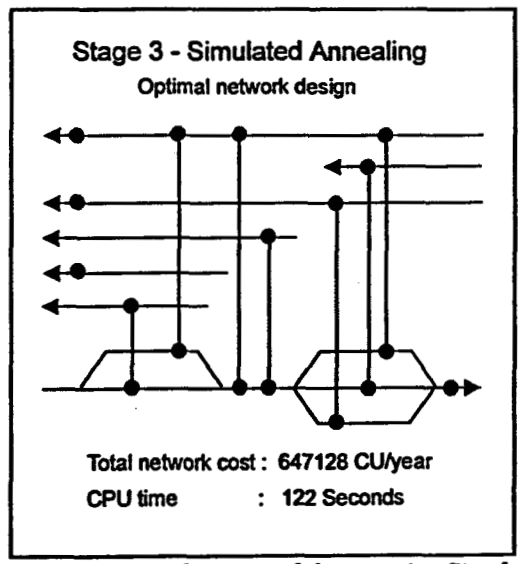


Figure 5.3 Final optimized design using Simulated Annealing with the initial MILP network.

A) Simulated Annealing stand alone with full model.

B) MILP, Simulated Annealing simple model, Simulated Annealing full model.

C) MILP, Simulated Annealing full model.

The result of keeping the network proposed by the simple model and only apply the new model is a cost increase to 660845 CU/year. If the full model is used with a stand alone Simulated Annealing algorithm an optimum network is found with an average cost of 655710 CU/year (CPU ca. 4600 sec.). With option B) an average cost of 657614 CU/year is found (CPU 125 Sec). Finally option C) gives 655900 CU/year within 650 sec.

The second example is a 5 stream problem with three cold and two hot streams. Stream and cost data are given in Table 3. Again a stand alone approach is applied. The results are given in Table 4. To get a result with a reasonable standard deviation it must be expected to use approaximately 800 seconds. With the combined approach using Pinch targeting, a simple MILP and Simulated Annealing a reasonable result was obtained within the range of 20 seconds. Again the combined approach shows an order of magnitude improvement to the stand alone approach.

	T-start K	T-target K	CP kW/K	h kW/m²/K
C1	311	478	11.3936	1.704
C2	339	455	12.9233	1.704
C3	366	478	13.0288	1.704
H1	522	394	16.6157	1.704
H2	478	339	13.2926	1.704
Steam	509.1	509	-	1.704
CW	311	312	-	3.417

Exchanger cc :	$145.65 * Area^{0.6}$ CU/year
Steam cost :	37.7879 CU/kW/year
CW cost :	18.1271 CU/kW/year

Table 3 Process streams and cost functions for example 2.

CPU Time	Average result	Approximate deviation
70	40200	2000
150	39300	400
800	39100	150

Table 4 Stand alone results for example 2 using a Simulated Annealing algorithm.

Discussion

The results from the examples show that there is a potential gain in applying different technologies to the problems in a coordinated way. The results indicate a considerable improvement of computational time and ability to handle problems with complex models. The question still remains at what levels to shift technologies. With a look at the combined design engine (Figure 6) it is noted that different paths can be chosen. Different designers will probably choose different paths dependent on their preference, experience, availability of software and of course the nature of the problem. The efficiency of each engine is of course very dependent on the designer. Nevertheless the benefits of combining technologies are obvious and should be enhanced.

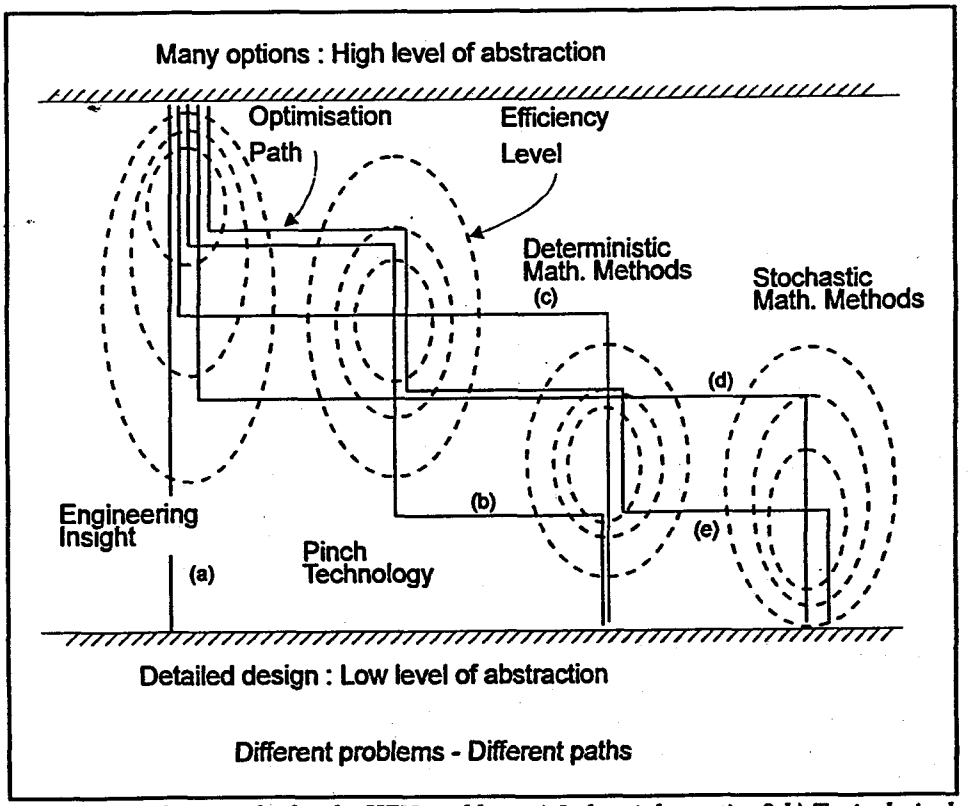


Figure 6 Synthesis paths for the HEN problem. a) Industrial practice ? b) Typical pinch based approach c) and d) Typical Mathematical approach e) Balanced combined approach.

Conclusion

A new framework for Heat Exchanger Network Synthesis is proposed. The new framework is based on a combined use of different technologies in a coordinated manner. The framework also includes a new enhanced representation of the Heat Exchanger Network using an object oriented approach.

The combined approach show that an order of magnitude computational time can be saved and that different levels of complexity can be handled systematically.

References

Ahmad S. and R. Smith, Targets and Design for minimum Number of Shells in Heat Exchanger Networks. *Chem Eng Res Des*, **67**, 481 (1989).

Dhole V.R. and B. Linnhoff, Distillation Column Targets, *Comp & Chem Engng*, **17**, 549 (1993).

Dhole V.R. and J. P. Zheng, Applying Combined Pinch and Exergy Analysis to Close Cycle Gas Turbine System Design, *ASME Cogen Turbo Power Conference*, Bournemouth UK (1993).

Gundersen T. and I. E. Grossmann, Improved optimization strategies for automated heat exchanger network synthesis through physical insights, *Comp & Chem Engng*, **14**, 925 (1990).

Kokossis A. C., Mathematical Programming Approaches in the Context of Process Integration, *10th Annual Consortium Meeting, Dep. of Process Integration*, Manchester October (1993).

Linnhoff B., Pinch Technology for the Synthesis of Optimal Heat and Power Systems, ASME Winter Meeting, Anaheim, AES Vol 2-1 (1986).

Linnhoff B., Pinch Analysis - A State-of-the-Art Overview, *Trans IChemE*, **71**, 503 (1993).

Smith R. and P. S. Jones, The Optimal Design of Integrated Evaporation Systems, *Heat Recovery Systems & CHP*, **10**, 341 (1990).

The American Society of Mechanical Engineers

Reprinted From
AES-Vol. 35, Thermodynamics and the Design, Analysis, and Improvement of Energy Systems
Editor: Robert J. Krane
Book No. H01045 – 1995

IMPROVED SYNTHESIS OF THE NITRIC ACID PROCESS

Jan Sandvig Nielsen and Mogens Weel Hansen
Department of Energy and Process Optimization
dk-TEKNIK
Copenhagen
Denmark

ABSTRACT

This paper introduces a new process concept for the nitric acid process that improves the exergetic efficiency of the process. Further it introduces and illustrates a general synthesis method that allows a fast and efficient evaluation of different process concepts. The conventional as well as the new nitric acid process is optimized using the proposed approach. Comparison is made on basis of the detailed process description given by Gaggioli et al. (1991) and Linnhoff and Alanis (1991) in their competition between *Exergy* and *Pinch* analysis. Energy efficiency is meassured in net power surplus for the process.

Where optimum performance for a conventional process is approximately 175 kWh/t(HNO_3) it is found to be approximately 230 kWh/t(HNO_3) with the new process. Another but equally important feature is that no steam cycle is necessary and thus an expensive steam turbine can be saved. If the saturated cycle is combined with a steam cycle it is possible to enhance the efficiency to 261 kWh/t(HNO_3).

DESIGN TECHNOLOGIES AND PERSPECTIVES

Thermodynamics provides an approach for identifying promising process heat recovery potential. The thermodynamical approach is based on a combination of engineering insights and visualization of the heat transfer between process streams. It is mainly based on identifying the thermodynamical inefficiencies within a given heat exchange system. The most successful use of these principles is the Pinch Technology, which enables the designer to predict the energy and capital targets ahead of design and get guidelines on how to achieve these targets. Since the late 70s pinch technology has been developed by Linnhoff and coworkers at UMIST as a complete methodology, which enables the fundamental understanding of the problem and reduces its combinatorial nature by applying targeting and decomposition. At the time Pinch Technology emerged it was focused on heat exchanger networks. The scope today includes separation system (Smith and Jones 1990, Dhole and Linnhoff 1993), heat and power integration (Linnhoff 1986,Linnhoff and Alanis 1991, Dhole and Zheng 1993) etc. The technology has moved toward a general targeting method and can be applied as a tool for screening and scoping among different process alternatives. The shift toward process analysis and targeting rather than design makes it natural to refer to the method as Pinch Analysis rather than Pinch Technology (Linnhoff 1993). Pinch Analysis is a well-tested approach which is able to provide information and guidelines to the designer at a high abstraction level. Although Pinch Analysis is able to screen among several alternative process alternatives it is less efficient when selecting between few competitive alternatives. In other terms, Pinch Analysis is efficient for high level decisions but cumbersome for detailed analysis.

Mathematical methods on the other hand offer a systematic evaluation of detailed alternatives. Mathematical programming approaches have established a methodology which is based upon the development of a reducible system representation inclusive of all possible design scenarios. The representation, known as superstructure or hyperstructure of the problem, is further modeled and optimized using algorithmic techniques. However, because a superstructure (or hyperstructure) is generally comprised by units and streams whose number increase combinatorial with the size of the problem, the mathematical programming approaches face an exponentially increasing computational burden in embracing more structural and operational alternatives. The situation, formally described as a NP-hard problem, imposes limitations on the methodology and the availability of appropriate solvers. The presence of discontinuities and complex nonlinearities makes it difficult to use off-the-shelf optimization procedures. To make the task practicable most methods are based on decomposing the

problem into minor problems with the subsequent risk of getting caught in a topology trap.

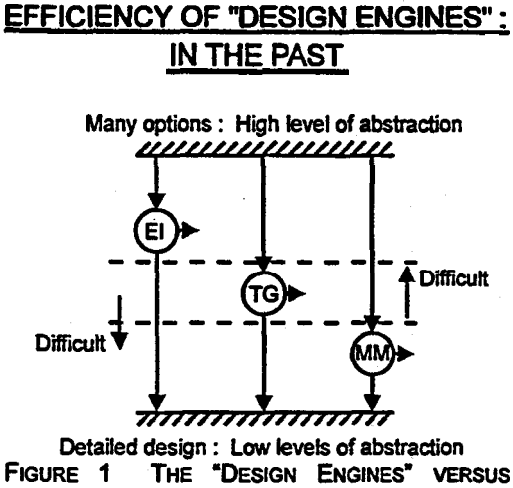


FIGURE 1 THE "DESIGN ENGINES" VERSUS ABSTRACTION.

A special branch of mathematical methods is the stochastic methods. These methods, who's origin should be traced in the analysis and optimization of clusters, are based on random search methods. They are to some extend insensitive to the discontinuities and complex nonlinearities. They are thus less exposed of getting caught in local optima. The stochastic methods can handle all sorts of complexity and are not dependent on gradients. They are therefore well-suited for combinatorial problems. The positive features of stochastic methods are all of a cost in computational efficiency. With no algorithmic or physical insights the stochastic methods will become costly in terms of computational efforts.

so far no systematic effort has been made for their integration. Instead we have seen that the different approaches have been extended to cover all levels of abstraction. In addition to the lack of integrated analysis to address the problem there are also important industrial aspects that are often disregarded to make the particular technology applicable and/or efficient. Among the frequent assumptions are those of constant heat capacity, countercurrent heat exchange, differentiable cost functions. Gundersen and Grossmann (1990) described the situation: With over 200 publications most of which in the last 8 years "It may come as a surprise that important design issues have not yet been adequately addressed and solved". The surprise reflects on the industrial experience where current practice is based on engineering experience and insight and to some extend on Pinch Analysis. There is only limited use of detailed design methods. This is probably because the problems are oversimplified and because the lack of flexible and efficient tools. What is needed are integrated approaches that better address the industrial problem.

DESIGN INTEGRATION SCHEMES

The different design technologies can be put in perspectives for integration schemes (Kokossis 1993, Nielsen et al. 1994). At the highest level engineering insights are used for a preliminary screening and decomposition with regard to process hierarchy. At an intermediate level targeting methods set goals. Finally at the low level mathematical methods perform detailed optimal designs. These technologies are set in perspective by viewing the approaches as "Design Engines" working between levels of abstraction (Figure 1). Engineering Insight (IE) delivers work with high efficiency at high level. If the approach is applied at a more detailed level difficulties will arise. The targeting methods (TG) deliver good work at the intermediate level but face difficulties at the high level as well at the low level. Finally Mathematical Methods (MM) deliver work with high efficiency at the low detailed level, while it has

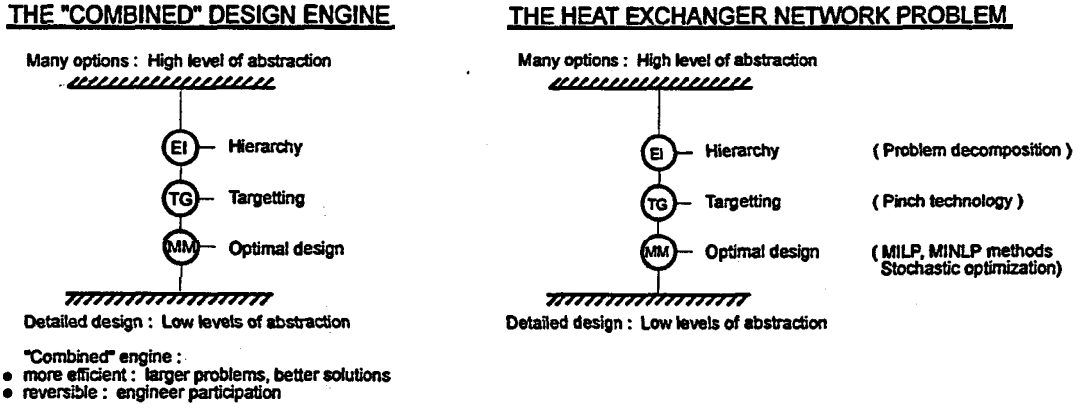


FIGURE 2 THE COMBINED DESIGN ENGINE. USING TECHNOLOGIES AT LEVELS WHERE OPTIMUM EFFICIENCY IS OBTAINED.

All of the above approaches have produced good solutions on different problems. Each approach seems to have its advantages and limitations. Moreover, there are apparent complementary features among these technologies in terms of potentials and limitations. But difficulties in delivering work at high abstraction level. In the past different schools have tried to extend their methods to cover all levels of abstraction. Figure 1 clearly impose that this is not an efficient use of technologies. What is proposed here is a "combined

design engine" that coordinates the effort in a way that give maximum efficiency at each level and allow for full engineering participation. The general approach is perfectly applicable to the heat exchanger network problem, where it is proposed to start with a hierarchical decomposition in order to initialize the problem (deriving process streams). As a next step a targeting method such as Pinch Analysis is proposed and finally mathematical methods are applied for detailed optimization (Figure 2). The combined approach utilizes the potential of each one of the approaches as well as minimize the limitations.

COMMERCIAL NITRIC ACID PRODUCTION

The nitric acid plants have attracted much attention because of their low second law efficiencies. The interest has further been enhanced by the competition between two different approaches. The *Pinch Analysis* proposed by Linnhoff and Alanis (1991) and *Exergy Analysis* by Gaggioli et al. (1991). In their respective studies the objective was to integrate a new plant with an on site steam power plant. In this paper it is only the nitric acid plant that is examined. Most contractors offer plants that are either steam exporting or power exporting (or both). In this paper the objective is to maximize the net power output with no steam export or import.

The commercial manufacture of HNO_3 of concentration up to 67% involves the following three main reactions:

$$4\ NH_3 + 5\ O_2 = 4\ NO + 6\ H_2O \quad (1)$$

$$2\ NO + O_2 = 2\ NO_2 \quad (2)$$

$$3\ NO_2 + H_2O = 2\ HNO_3 + NO \quad (3)$$

The NO in the product stream is stripped and recycled. This give a net reaction of

$$NH_3 + 2\ O_2 = HNO_3 + H_2O \quad (4)$$

A considerable amount of heat is released (420.45 KJ/mole) by the above reaction. Part of this heat is converted into mechanical work to drive compressors in the process. The base case used by Linnhoff and Alanis (power output mode) was a 890 tpd (100% HNO_3) unit with a net power export of 3965 kW (Figure 3). This gives a specific production of 106 kWh/ton(100% HNO_3). It is, however, a base case that is *not* state of the art. This is reflected by the fact that Kemira's HNO_3 unit IV (UHDE design licensed 1979) has a specific output of ca. 124 kWh/ton(100% HNO_3).

BASE CASE

This case was originally presented by Linnhoff during a conference in 1987 (Gaggioli et al. 1991). It was the purpose that the case should be used in a challenge between the school of Exergy Analysis represented by Gaggioli et al. (1991) and the school of Pinch Analysis (Linnhoff and Alanis, 1991). The dual pressure nitric acid plant is showed in Figure 1 with the detail of flows, compositions, and thermodynamic properties associated with each streams in table 1. Further the compressor and turbine efficiencies are given in table 2. These values are calculated from the stream properties in table 1. Finally a set of constraints is assumed. It is in this case study assumed that the reaction conditions should be considered fixed. This means that the converter temperature should be kept on 840 °C and the pressure 3.3 bar. The oxidization heat is released linearly in the temperature interval imposed by table 1.

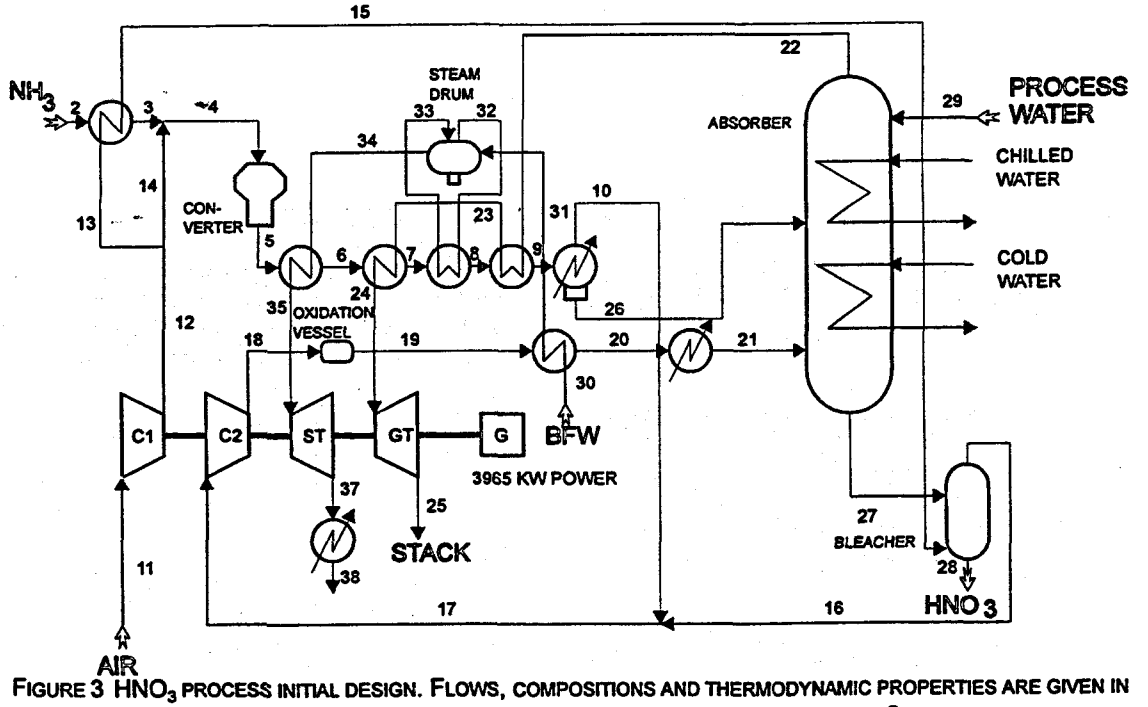


FIGURE 3 HNO_3 PROCESS INITIAL DESIGN. FLOWS, COMPOSITIONS AND THERMODYNAMIC PROPERTIES ARE GIVEN IN TABLE 1. ISENTROPIC EFFICIENCIES FOR TURBINES AND COMPRESSORS ARE GIVEN IN TABLE 2.

Flow	T	P	Flow						H(T,P)
	°C	Bar	Kg/hr						kW
			N2	O2	H2O	NH3	NO	NO2	
2	7	5.5				10679.8			-174
3	76	5.5				10679.8			279.6
4	170	3.5	126152.7	38311.2		10679.8			7857.6
5	840	3.3	126504	13627.8	16946.3		18064.4		47259.7
6	763	3.3	126504	13627.8	16946.3		18064.4		42495.6
7	592	3.3	126504	13627.8	16946.3		18064.4		31994.6
8	325	3.3	126504	13627.8	16946.3		18064.4		16466.1
9	135	3.16	126504	11412.3	16946.3		13909.6	6370.4	5842.8
10	50	3.16	126504	3995.3	931		1538.6	20616.1	1030
11	20	1	141519	42993					-278
12	184	3.5	141519	42993					8272
13	184	3.5	126152.7	38311.2					7378
14	184	3.5	15366.3	4681.8					894
15	103.5	3.5	15366.3	4681.8					440.4
16	67	3	15366.3	4681.8					233.6
17	52	3	141870.3	8677.1	931		1538.6	20616.1	1267.8
18	224.5	10.25	141870.3	8677.1	931		1538.6	20616.1	9823
19	236	10.25	141870.3	8172.8	931		592.9	22066	10380.5
20	156	10.25	141870.3	8172.8	931		592.9	22066	6377
21	43	10.25	141870.3	8172.8	931		592.9	22066	713.7
22	18	8.9	141870.3	3877	383		15	23	-491.9
23	297	8.9	141870.3	3877	383		15	23	11766.6
24	536	8.9	141870.3	3877	383		15	23	22267.7
25	243	1	141870.3	3877	383		15	23	9237.7
			H2O	HNO3					
26	50	3.16	15078	6462					457.1
27	41	3	36013.4	37865					907.1
28	45	3	36013.4	37865					1114
			H2O(L)	H2O(G)					
29	20	10	24678						-143.3
30	20	80	30036						2604.8
31	194	80	30036						6050.6
32	295	80	38794.3						13063
33	295	80		38794.3					28591.4
34	295	80		30036					22136.6
35	473	80		30036					26900.6
37	50	0.1233	2842.7	27193.3					18865.7
38	50	0.1233	30036						871.8

TABLE 1 HEAT AND MASS BALANCES OF A DUAL PRESSURE NITRIC ACID PLANT (GAGGIOLI ET AL. 1991).

Finally the tail gas inlet temperature to the expander is limited to 700 °C. Some of these constraints can be discussed, but so far they can be viewed as safe side constraints and will be used in this case study.

There are several different paths for improving the net power output from the process plant. In the studies of the above mentioned authors basically two parameters are examined

a) Increased gas turbine temperature.
b) Increased steam production.

The optimum is then found as a combination of the two parameters. Associated with option b) minor changes in pressure have been included. Optimization of the power production with these options can be done in two steps using the principle of pinch analysis

1) Targeting
2) Design

	Air compressor C1	NO compressor C2	Tail gas turbine GT	Steam turbine ST
Isentropic efficiencies	76.0	75.5	81.0	72.0[1]

TABLE 2 ISENTROPIC EFFICIENCIES FOR TURBOMACHINERY CALCULATED FROM TABLE 1.

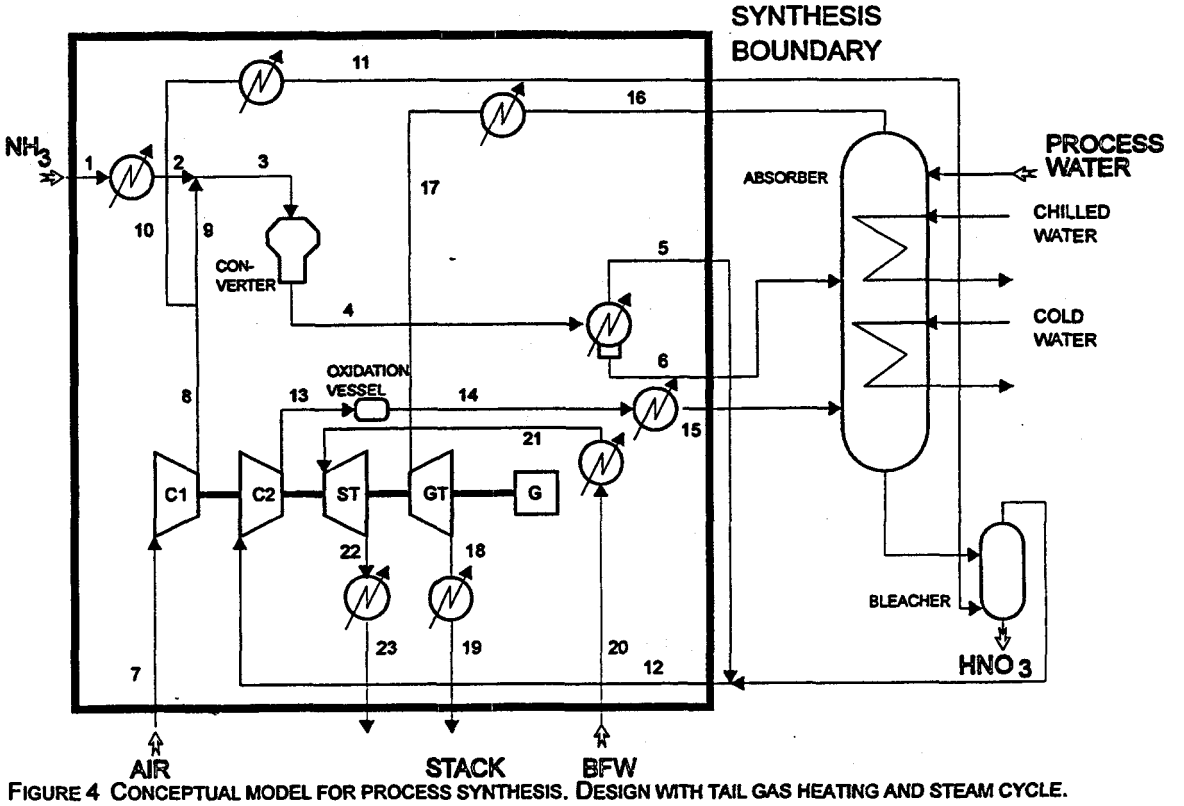


FIGURE 4 CONCEPTUAL MODEL FOR PROCESS SYNTHESIS. DESIGN WITH TAIL GAS HEATING AND STEAM CYCLE.

With the energy targeting procedure from pinch analysis it is possible to predict the minimum energy consumption for a given heat recovery problem under the assumption that all streams are known in priori. The energy targeting, however, has little meaning in the case of the nitric acid process because no additional heat supply is desirable. The targeting procedure can instead be used to determine the minimum approach temperature. For the base case the minimum approach temperature is found to be approximately 57 °C. A way to utilize the targeting method in Pinch Analysis is to remove all internal heat exchangers and replace them with utility heaters and coolers. This gives a simplified conceptual simulation model (Figure 4).

With the conceptual model it is possible to write down a strategy for power production improvement which in its general form can be written as

1. Change power related streams (steam flow rate, tail gas temperature etc.).
2. Check that the process to process heat transfer is feasible and get minimum approach temperature.
3. Repeat 1 and 2 until sufficient approach temperature is found.

With this simple strategy it is very simple to evaluate the different options. The simulator gives the resulting power output while the pinch targeting will check for feasibility. The composite curves can be used as to identify exergy improvement direction. There is at this stage no need to design the actual heat exchanger network.

In the targeting part it has been decided to use 20 °C and 40 °C as minimum temperature approaches. The above approach has been used to find the optimal power production using the following options.

[1] The steam turbine efficiency include wetness and exhaust end loss which are assumed constant and independent of final moisture content in the steam turbine

No	Tail gas	Steam		Power output	ΔT_{min}
	Temp. °C	Pressure bar	flow kg/h	kW	°C
Base Case	536	80	30036	3971	57.3
A1	600	100	35200	5534	19.7
A2	600	100	32000	4756	40.3
A3	650	100	33700	6011	19.8
A4	650	100	29900	5088	40.0
A5	700	100	32200	6492	19.7
A6	700	100	26250	5046	40.2
A7	750	100	30600	6952	19.9
A8	750	100	24600	5494	39.8

TABLE 3 PERFORMANCE OF THE OPTIMIZED CONVENTIONAL NITRIC ACID PROCESS.

Tail gas temperature	500 - 700 °C (750 °C)
Steam pressure	80 - 100 bar
Steam flow rate	free

A look at the process composite curve (figure 3) for the base case shows a clear potential for both tail gas temperature rising and/or steam increase.

It has been chosen to limit the tail gas temperature to 700 °C in this study. It is, however, easy to evaluate the effect of this constraint using the proposed strategy. The result of several configurations is listed in table 3. From the targeting/simulation result it can be concluded that the best configuration is with maximum tail gas temperature and maximum steam pressure. With the limit set in this study this give an optimal conceptual

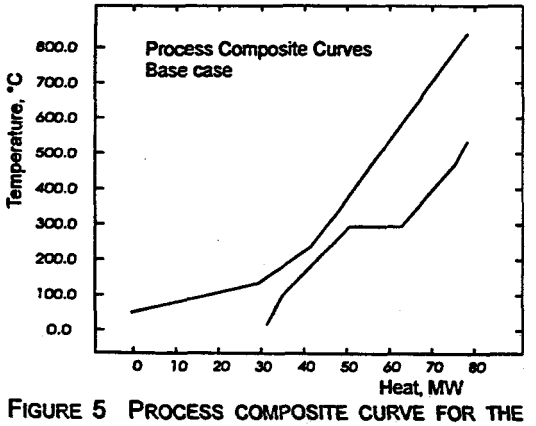


FIGURE 5 PROCESS COMPOSITE CURVE FOR THE NITRIC ACID BASE CASE AS GIVEN BY LINNHOFF AND ALANIS (1991).

design with a tail gas temperature on 700 °C and a steam cycle with a flow of 28,641 kg/h (ΔT_{min} = 20°C) and 100 bar. A process with these design values will give a power output of 6492 kW (174 kWh/ton). It can be noted that if we relax the constraint on the tail gas temperature to 750°C, the process will be able to deliver 6952 kW (186 kWh/ton).

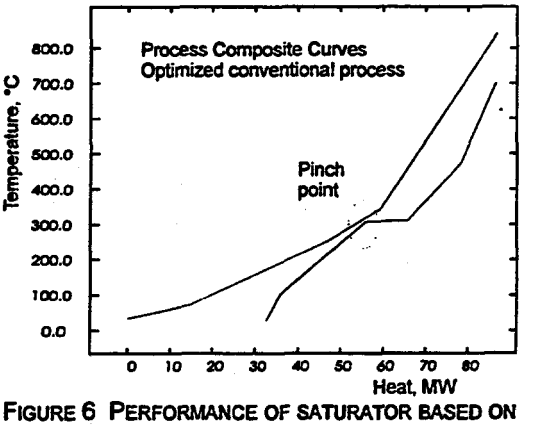


FIGURE 6 PERFORMANCE OF SATURATOR BASED ON 180 °C WATER. THE TAIL GAS FLOW RATE IS 146,168 KG/H.

TAIL GAS SATURATION

One of the major sources of exergy loss in the nitric acid plant is the excessive temperature driving forces at the high temperature level. Even after optimzation of the conventional process is there considerable driving forces (Figure 6). The driving forces could be decreased by increasing the massflow of the heated tail gas. In this paper we propose to saturate the tail gas leaving the absorption column using heated water. A similar concept is well-known from the HAT power cycle (e.g., Rao 1989). The effect of saturating the gas with hot water is twofold - an increased massflow rate and an increased temperature. The mass transfer is increasing with water temperature and flow rate. This is quantified in Figure 5 where the tail gas is saturated using an absorption column model.

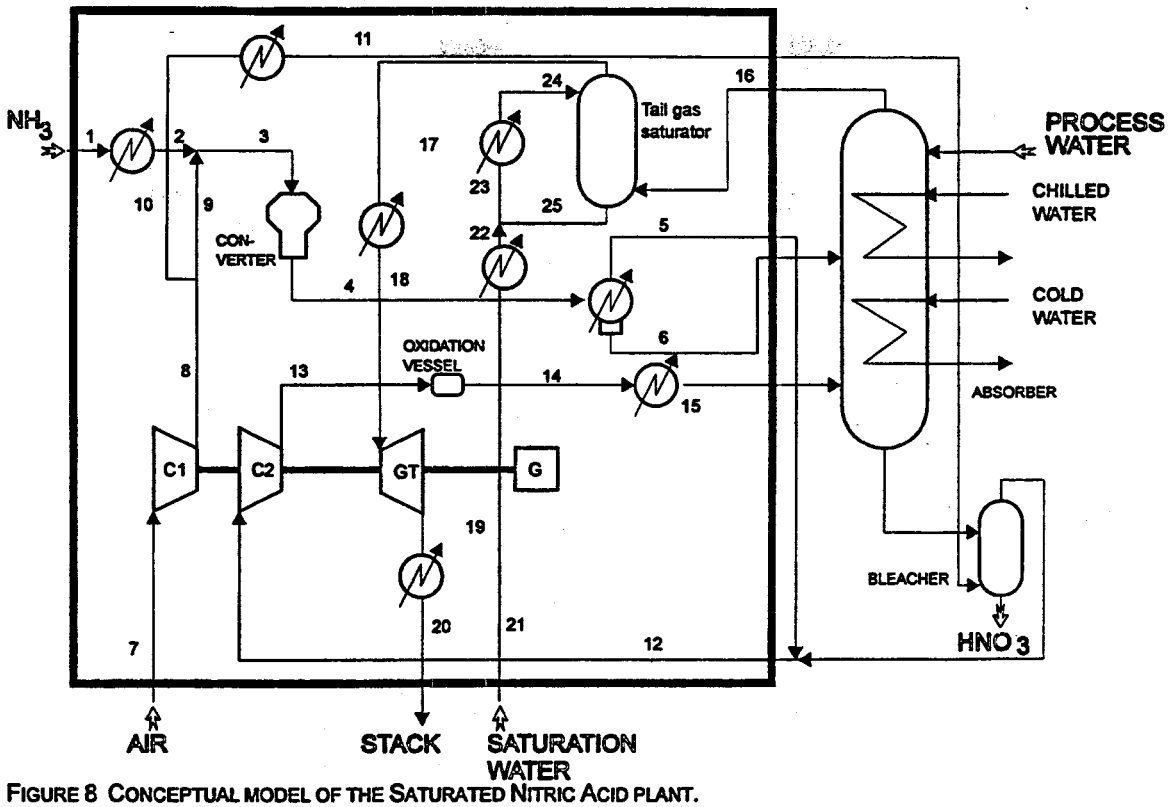


FIGURE 8 CONCEPTUAL MODEL OF THE SATURATED NITRIC ACID PLANT.

Using the properties for the tail gas in table 1, the performance of the saturator is simulated using HYSIM process simulation software. It is possible to double the total flow of the tail gas if enough hot water is used. The hot water must be produced using the heat from the process. To avoid exergy loss the heating is done in two steps. The fresh water is heated to the saturator outlet temperature and then mixed with the water leaving the saturator. Finally the total water flow is heated to the inlet condition. The saturator can be integrated with the process using the same strategy as before. We assume that all heating demand is handled with hot utilities and all cooling demands with cold utilities. This gives a new conceptual model of the process which is showed in figure 6. It can be noticed that the steam cycle has been removed.

The key parameters for optimization are in this case

Saturator water flow
Saturator water temperature
Tail gas temperature

The maximum temperature of the saturation water is set to 180 °C. This limit is chosen to be reasonable working with a saturation water cycle on 12 bar.

TARGETING METHOD FOR TAIL GAS SATURATION

The conceptual model (Figure 8) can be simplified further by using a targeting method for tail gas saturation. In the saturation tower a simultaneous mass and heat transfer takes place. The associated heat is delivered from the process to the two water heaters. These heaters represent the heat necessary for the saturator. An alternative model could be used to represent the

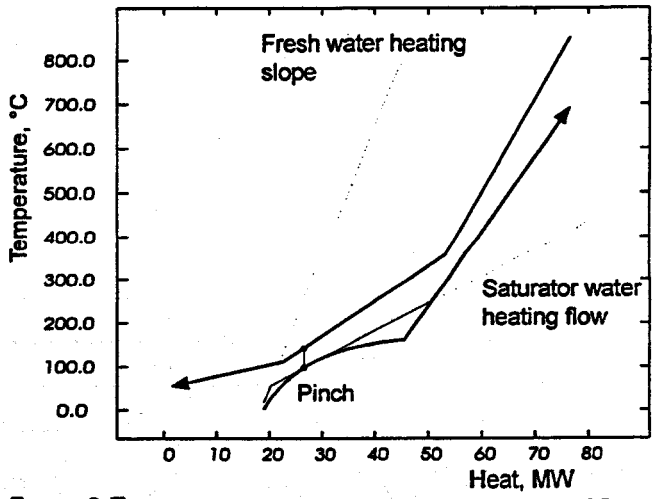


FIGURE 9 TARGETING MODEL FOR SATURATOR PERFORMANCE.

heating requirement. In that model a given amount of fresh water is mixed with the tail gas giving a two-phase flow. The mixture is then heated to the gas turbine temperature. The water gradually evaporates until all water is evaporated. The heat curve for heating is shown in Figure 9. The benefit in using this alternative model is a simplification in the synthesis. One of the optimization parameters (saturator water temperature) can be removed.

Case	Turbine inlet temperature °C	Saturator mass transfer kg/h	Power output kW	ΔT_{min} °C
B1	600	59400	6370	20.3
B2	600	55000	5676	40.2
B3	650	57700	7505	20.3
B4	650	53400	6786	40.0
B5	700	56000	8612	20.4
B6	700	51800	7868	40.1
B7	750	44000	7765	20.1
B8	750	38000	6643	39.9

TABLE 4 PERFORMANCE OF THE OPTIMIZED SATURATED NITRIC ACID PROCESS.

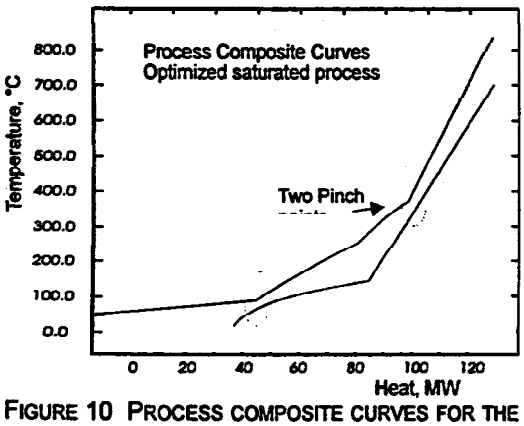


FIGURE 10 PROCESS COMPOSITE CURVES FOR THE OPTIMIZED SATURATED PROCESS.

PERFORMANCE OF THE SATURATED NITRIC ACID PROCESS

The proposed modified nitric acid process is optimized using the conceptual model with saturator targeting. The results are, as for the conventional process, obtained with 20 °C as well as 40 °C. With the conceptual model the degree of freedom is cut down to two - tail gas temperature and added water flow. It is thus straight forward to optimize the process iteratively using a standard process simulator (HYSIM). In this case the optimum amount of water is found for a rangeof fixed turbine inlet temperature. The results are given in table 4. An interesting feature of the new process is that it exhibits an optimum tail gas temperature at 700 °C. There is in this case no benefit in relaxing the temperature constraint. With ΔT_{min} at 20 °C the proposed process yields 8612 kW (230 kWh/ton) which is 33% better than the optimized conventional process.

Case	Turbine temperature °C	Saturator mass transfer kg/h	Steam production kg/h	Power output KW	ΔT_{min}
C1	600	34500	24500	8395	19.7
C2	600	34900	22000	7519	40.0
C3	650	37000	20600	9045	19.7
C4	650	39500	15300	7944	39.8
C5	700	37500	19500	9778	20.0
C6	700	42000	9500	8440	39.7
C7	750	38000	17000	10518	19.9
C8	750	33000	18500	9257	40.4

TABLE 5 PERFORMANCE OF THE EXTENDED SATURATED NITRIC ACID PROCESS.

It is quite simple to retrieve the full model from the targeting model. This can be done graphically - Figure 9. The slope of the fresh water heating is determined by the amount of fresh water. The best heating of the rest can be determined by looking at the saturation curve along with the process heat release curve. If the pinch is located at the saturation curve the line has to be drawn through the pinch point in order to maintain the minimum approach temperature.

FURTHER IMPROVEMENTS?

So far the optimization has been done in a practical spirit. The technology in the new process is from an economical point of view competitive with the traditional process. In the new process an absorption column and additional heat transfer equipment replace the steam turbine which is a high capital cost equipment.

An alternative to the Saturated process is a process with more than one steam pressure. As a practical extreme we have chosen to optimize the plant using three steam pressure levels (100, 12 and 1 bar) with associated steam turbines. With the same conditions for the core process (Table 1) this gives a net power output of 8819 kW (235 kW/t(HNO_3) at ΔT_{min}=20°C.

It is also possible to boost the Saturated Process by including a steam cycle. The extended Saturated Process is optimized using an 100 bar steam cycle. The results are given in table 5. With the 700 °C constraint on turbine temperature a new optimal power production is found to 9778 kW (261 kWh/ton) with ΔT_{min} = 20°C. For each gas turbine inlet temperature the optimum configuration is found when two pinches occur simultaneously. ne pinch caused by the steam raising and one by the saturation water heating.

The extended Saturated Process thus delivers about 11 % more power than the multi steam pressure process. The estimated equipment cost will probably be considerable lower for the new process compared with the multi steam level process.

HEAT EXCHANGER NETWORK DESIGN

Until now all evaluations have been done at a conceptual level, not taking into account the specific heat exchanger network. It has been assumed that a minimum approach temperature should be maintained. This value should represent the correct energy capital tradeoff.

To investigate the difference in heat exchanger network design among the concepts, two networks will be designed. One for case A5 and one for case B5. The networks are synthesized with the program *HEN Explorer* (Nielsen 1995). It is assumed that the cost function follows:

The resulting networks are showed in Figure 11.

The additional heat exchanger cost for the saturated process

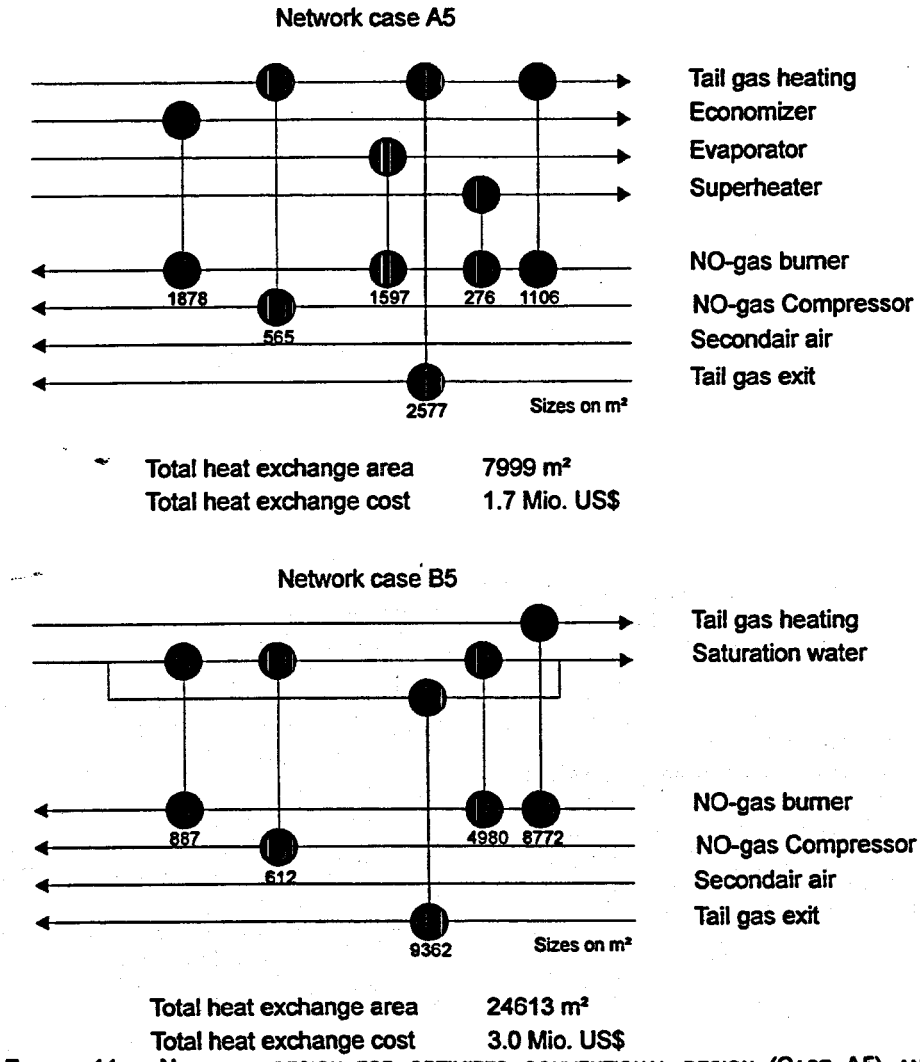


FIGURE 11 NETWORK DESIGN FOR OPTIMIZED CONVENTIONAL DESIGN (CASE A5) AND OPTIMIZED SATURATED DESIGN (CASE B5).

compared with the conventional process is thus 1.3 10^6 US$. Compared with the huge increase in power output and the fact that the steam turbine is removed this additional cost seems to be quite small.

TURBO MACHINERY EFFICIENCIES

For comparison the different process concept has been evaluated for the same equipment efficiencies as imposed by table 2. These efficiencies are, however, lower than those available for new plant design. Better understanding and advanced aerothermodynamic modeling of compressors and expanders have lead to a dramatic increase in turbo machinery within the last decades. Modern gas turbine system thus operates with *polytropic efficiencies* for compressors of approximately 88% to 91% and for expanders 83% to 88%.

For the steam turbines used in this study the adiabatic efficiency of 72% seems to match reasonablely with the values of those machineries delivered in the last decade or so. Under the conditions used in this study a typical exhaust end loss and moisture loss will each be approximately 2.5%. When the steam turbine is downsized, as with the boosted saturated cycle, these losses will increase. Therefore, in that particular case a reasonable adiabatic efficiency will be approximately 67%.

To see the effect of increasing efficiency optimization has been

	Air compressor C1	NO compressor C2	Tail gas turbine GT	Steam turbine ST
Polytropic efficiency	89	86	85	
Isentropic efficiency	87	83	88	72.0[2]

TABLE 6 UPDATED TURBO MACHINERY EFFICIENCIES.

carried out with the adiabatic efficiencies given in table 6.

With these value the optimization can be revised, which is done for max gas turbine inlet temperature (700°C) and ΔT_{min}=20°C (Table 7).

CONCLUSION AND SIGNIFICANCE

This study has demonstrated how a top down analysis of a given process can give considerable improvements in energy efficiency. By using a structured approach that takes advantages of different design technologies (Heuristics, Exergy, Pinch and mathematical methods) a new concept for energy efficient nitric acid production has been evaluated and optimized.

[2] 72% for large steam flow and 67 for small steam flow.

Gross power output kW	Conventional design A5	Saturated design B5	Multi steam leveldesign	Enhanced saturated design C5
Table 2 efficiencies	6492	8612	8819	9778
Table 6 efficiencies	8679	11826	10927	12341

TABLE 7 PERFOMANCE IMPROVEMENT USING STATE OF THE ART EFFICIENCIES.

This has resulted in a improvement in specific power production from 171 kWh/t(HNO_3) to 258 kWh/t(HNO_3) using conservative equipment efficiencies as imposed by Linnhoff and Alanis (1991).

Using more appropriate turbo machinery, it has been showed that the proposed saturated nitric acid process is able to produce nitric acid giving a gross power output of 312 kWh/t(HNO_3) with no steam cycle and up to 326 kWh/t(HNO_3) with a small additional steam cycle.

Considering that today's nitric acid plants have a typical power output in the range 0 to 140 kWh/t(HNO_3), the new process has a good change of ousting the conventional nitric acid process, when it comes to new design.

REFERENCES

Dhole V.R. and B. Linnhoff, Distillation Column Targets, *Comp & Chem Engng*, **17**, 549 (1993).

Dhole V.R. and J. P. Zheng, Applying Combined Pinch and Exergy Analysis to Close Cycle Gas Turbine System Design, *ASME Cogen Turbo Power Conference*, Bournemouth UK (1993).

Gaggioli R.A., D.A. Sama, S. Qian and Y.M. El-Sayed, Integration of a New Process Into an Existing Site - A Case Study in the Application of Exergy Analysis, *ASME Journal of Engineering for Gas Turbines and Power*, **113**, 170 (1991).

Gundersen T. and I. E. Grossmann, Improved optimization strategies for automated heat exchanger network synthesis through physical insights, *Comp & Chem Engng*, **14**, 925 (1990).

Kokossis A. C., Mathematical Programming Approaches in the Context of Process Integration, *10th Annual Consortium Meeting, Dep. of Process Integration*, Manchester October (1993).

Linnhoff B., Pinch Technology for the Synthesis of Optimal Heat and Power Systems, ASME Winter Meeting, Anaheim, AES Vol 2-1 (1986).

Linnhoff B. and F.J. Alanis, Integration of a New Process Into an Existing Site - A Case Study in the Application of Pinch

Technology, *ASME Journal of Engineering for Gas Turbines and Power*, **113**, 159 (1991).

Linnhoff B., Pinch Analysis - A State-of-the-Art Overview, *Trans IChemE*, **71**, 503 (1993).

Nielsen J.S., Optimization of Energy Systems by Simulated Annealing; ASME Winter Annual Meeting 1993, AES-Vol. 30 (1993).

Nielsen J.S, V. Briones-Vallejo and A.C. Kokossis, An Integrated Framework for the Optimal Design of Heat Recovery Systems, Paper 225g AIChE annual meeting San Francisco November (1994).

Nielsen J.S., Integrated Optimization of Process Sites, Ph.D. Thesis Technical University of Denmark (1995).

Rao, A.D., Process for Producing Power, *US Patent 4,829,763* (1989).

Smith R. and P. S. Jones, The Optimal Design of Integrated Evaporation Systems, *Heat Recovery Systems & CHP*, **10**, 341 (1990).

Pergamon

Computers chem. Engng Vol. 20, Suppl., pp. S249–S254, 1996

S0098-1354(96)00052-X
0098-1354/96 $15.00+0.00

HEAT EXCHANGER NETWORK MODELLING FRAMEWORK FOR OPTIMAL DESIGN AND RETROFITTING

Jan Sandvig Nielsen[§], Mogens Weel Hansen[§§] and Sten bay Joergensen

Department of Chemical Engineering, Technical University of Denmark, DK 2800 Lyngby
[§] present address: [§§] dk-TEKNIK, Gladsaxe Moellevej 15, DK 2860 Soeborg

ABSTRACT

A new framework for addressing the practical industrial heat exchanger network (HEN) synthesis problem is presented. The new framework is based on a new object oriented representation of the HEN synthesis that allow handling of models of different complexity. To handle the increased complexity of the resulting optimisation problem a Simulated Annealing algorithm is adapted similar to that of Dolan et al (1989,1990). The proposed framework is implemented as the software tool HEN Explorer that successfully is tested on problems of varying complexity.

KEYWORDS

Heat Exchanger Network Synthesis, Industrial aspects, Simulated Annealing, Object Oriented Design

Introduction

HEN synthesis techniques have evolved tremendously during the last two decades (Grossmann and Kravanja 1995). There are however a number of issues that have not been efficiently formulated and solved. Most problems presented in literature are based on the assumption of countercurrent heat exchange. Therefore many solutions that feature an optimum approach temperature under 10 °C are not practically feasible. There are several other simplifications made that prevent a more wide spread application of HEN synthesis tools. Other assumptions frequently used (Grossmann 1993) are constant heat capacity flowrates, fixed inlet and outlet temperatures and neglecting of pressure drops. There is a good reason for these simplifications. Only recently methods have been developed for efficiently solving simplified HEN synthesis problem after decade's research efforts. This is mainly due to the complex nonlinearities and discontinuities present in the problem. It is therefore evident that adding new complexities to the problem formulation will create further problems for the solution procedures. A dual challenge have thus appeared: Create better HEN synthesis model and improve solution methodology. In this paper an object oriented modelling approach is combined with a Simulated Annealing algorithm (Kirkpatrick, 1983 and Dolan et al., 1989,1990) to comply with the stated challenge. The purpose of this paper is to present one solution to this dual challenge. The paper is organised as follows: First the new HEN synthesis framework is presented. Then a proposed strategy for solving the problem is presented. Subsequently two examples are presented and conclusion is drawn.

New HEN synthesis framework

To improve modelling capabilities the HEN synthesis framework is redesigned based upon the functional behaviour of all elements included in a HEN synthesis study. This new heat exchanger network modelling framework addresses the synthesis of practical industrial heat exchanger networks and treats grassroot as well as retrofit design. The methodology includes detailed heat exchanger modelling, non-constant heat capacities and heat transfer coefficients as well as flexibility and pressure drop considerations. The key element for development of such a framework is to treat each HEN component (streams, exchangers, pumps etc.) conceptually. Thus each element is described by its functional behaviour. From this conceptual description a set of generic elements describing the general functions of the network is derived. In the modelling procedure the heat exchanger network is split into two categories representing the connections (process streams) and the physical structure (HEN nodes) respectively. This generic HEN model is represented in an object oriented framework, where each element is treated as an individual object with its associated properties. Thus this new representation is an extension of Dolan et al's (1990) linked list representation. One major advantage obtained from deriving all network elements from a common base of generic units is that the new framework in a consistent way can handle models of different complexity.

A Simulated Annealing algorithm is adopted for solving the resulting HEN synthesis problem. The object oriented representation combined with the Simulated Annealing algorithm allows for synthesis of problems with a high degree of complexity and thus for handling problems met in industrial practice.

Heat exchanger modelling in the context of HEN Synthesis

For industrial application of HEN synthesis tools one of the most severe limitations is the assumption of ideal countercurrent heat exchange. In most literature problems the optimum operating point requires a minimum temperature difference ΔT_{min} less than 10 °C. This is the case with problem 7SP4 analysed by Floudas et al (1986) and later Dolan et al (1989,1990). In the solution of Floudas et al a decomposition strategy was used for prediction of the optimum ΔT_{min}. In their solution this was at ΔT_{min}=5.6 °C. Dolan found the so far best recorded solution by using a Simulated Annealing approach. Their solution is outlined in figure 1. It is noted that ΔT_{min} in the proposed network is 2.5°C. If a single pass 1-2 exchanger is used the resulting solution of Dolan et al becomes infeasible. Applying a multipass heat exchanger model the solution becomes feasible with a high number of shells. Using the design approach suggested by Ahmad et al. (1990) with a specified X_P = 0.9 one of the pinched exchangers will require 47 shells which is very unlikely to be accepted.

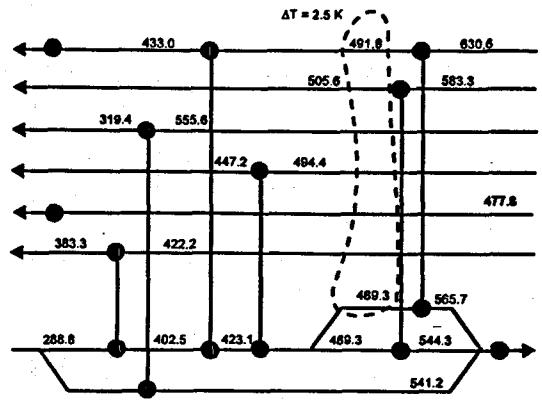


Figure 1. Optimum solution found by Dolan et al (1990) for the 7SP4 HEN synthesis problem prepared by Floudas et al (1986).

The new conceptual view of the heat exchanger modelling is outlined in figure 2 where the functionality of a heat exchanger network unit is conceptualised in a set of generic properties and methods. From an overall point of view all HEN units perform energy and mass balances and design calculations. The type of calculation is the same but the specific calculation is dependent of the specific type of operation. For heat exchanger units energy and mass balances are normally independent of the heat exchanger model while the design equations and costing equations typically vary considerably depending on exchanger type. This was clearly demonstrated with the example in Figure 1. In an object oriented hierarchical representation of the HEN unit models all units are derived from a single generic HEN unit model. All models in the object tree have embedded methods to perform mass and energy balances as well as design and costing calculations. To allow better matching of process streams it can be convenient to use stream splits and mixing. The same type of calculation can be performed as for the heat exchanger units and they thus can be derived from the same generic HEN unit model. It is also possible to include other HEN units that are not typically included in HEN synthesis studies like pumps and compressors. The only requirement is that these models include methods for performing energy, mass and sizing calculations. With the proposed framework the development is decomposed. From an overall point of view all possible HEN unit models respond on the same request although the specific action is taken care of by the specific models. In this way it is possible to enhance the modelling of specific operations without modifying the general overall model. In the current object tree different heat exchanger models is included for new design as well as for retrofit design. The most important feature is, however, the extendibility. It is easy to derive new modified heat exchanger models from the object tree.

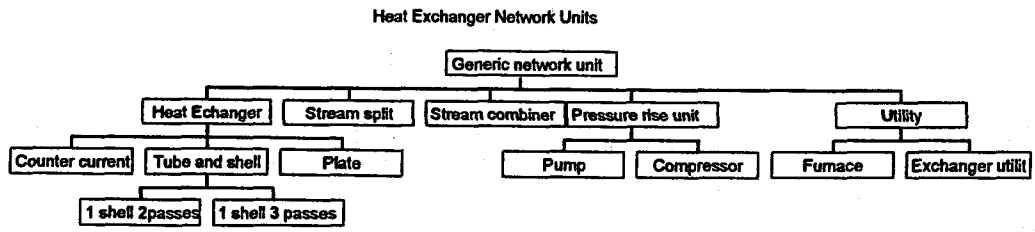


Figure 2. Heat Exchanger Network unit hierarchy.

Process stream representation.

A representation similar to that for the HEN units can be derived for the process streams. In most HEN synthesis methods it is assumed that heat capacity flowrate can be assumed constant. While this can be a reasonable approximation for constant composition process streams with no phase changes it can be a fatal assumption in other cases e.g. when fully or partial phase changes takes place. This is a typical situation in many industrial process plants. To illustrate the shortcoming of the simple formulation a humid air process stream is considered

(Figure 3). In figure 1a a humid air process stream is show along with the dew point curve. When the temperature is lowered below the dew point then part of the water will be condensed. In Figure 1b the resulting enthalpy-temperature curve for the cooling is shown together with a linearised enthalpy-temperature curve (constant heat capacity flow rate). In figure 1c a cold composite curve is added representing the streams that require heating. It is clearly seen that assuming constant heat capacity in this case can lead to the false conclusion that the humid air process stream can be utilised to below the dew point. Similar consideration goes for reactive process streams where reaction takes place during heating/cooling. This is e.g. the case in the Nitric Acid process where NO is oxidised to NO_2 under cooling. A simple way to resolve the problem using standard HEN synthesis procedure is to split process streams into minor process streams each with constant heat capacity flowrate. This method will however most likely result in a solution with to many heat exchangers.

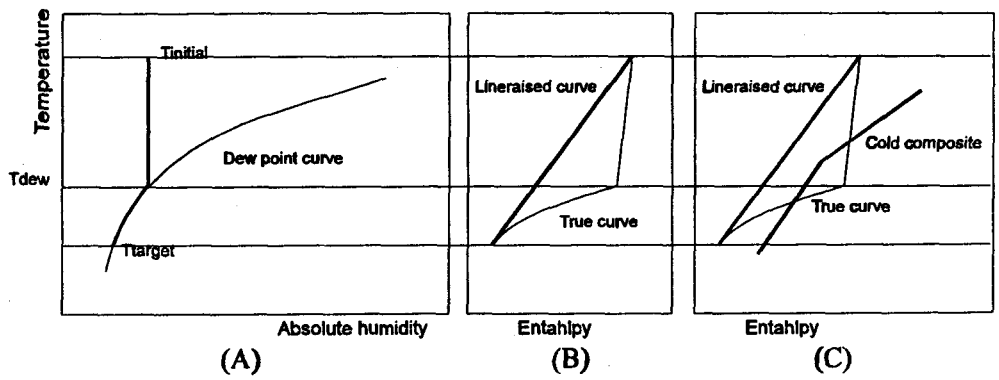


Figure 3. Fatal linearisation for humid air cooling.

The representation of process streams used in this work is based on an object hierarchy as for the HEN unit models. In this case each model has embedded methods for calculating temperature dependent properties (f.ex. temperature-energy relations). The simplest model in this hierarchy is a model for the constant heat capacity (and heat transfer coefficient). A more detailed model is the piecewise linearised model where the properties (heat capacity flowrate and heat transfer coefficients) are linearised over a finite number of temperature intervals. Finally a full property model can be applied using a standard property calculation model. As for the HEN unit models, stream models are independent of the overall model. The stream model hierarchy is outlined in Figure 4.

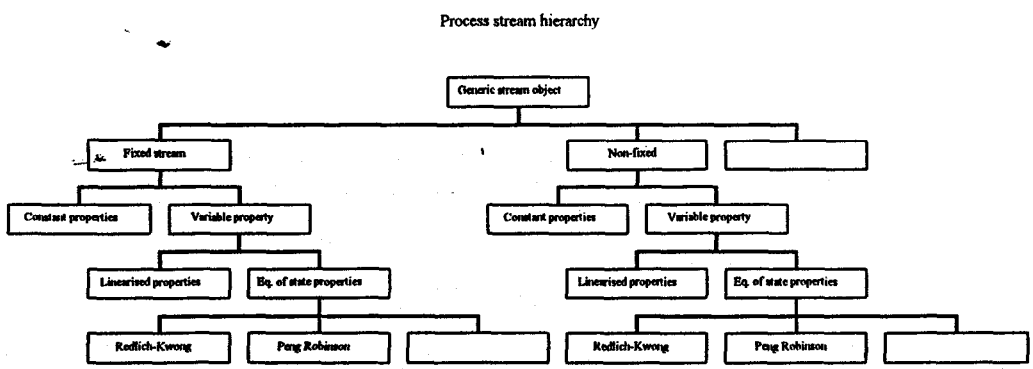


Figure 4 Process stream modelling hierarchy.

HEN Explorer

A software tool - HEN Explorer - is based on the conceptual framework described above. Currently a Simulated Annealing algorithm similar to that of Dolan et al. (1990) is implemented for complex optimisation. Implementation has been carried out to support model extendibility and flexibility. It is important that new modelling features can be included without changing the program structure. Further it is also desirable to have the ability to work with different levels of complexity within the same framework.

Two examples are presented to illustrate the enhanced features of HEN Explorer. The first example involves tube and shell exchangers while the second example is a retrofit study with variable properties.

EXAMPLE 1

This example is taken from Ahmad (1985) who suggest a method for designing minimum number of 1-2 shells in an exchanger based on a specified effectiveness parameter X_P. Problem data for this example is given in Table 1.

Stream	T-initial °C	T-target °C	M Cp kW/°C	h kW/m²°C
C1	120	235	2	0.4
C2	180	240	4	0.4
H1	260	160	3	0.4
H2	250	130	1.5	0.4
			Cost $/kW.yr	
CW	30	80	12.2	0.4
ST	280	279	110.0	0.4
Exchanger cost	300 $A^{0.5}$		$X_P = 0.9$	

Table 1. Example 1 (Ahmad 1985).

The result of using HEN Explorer is compared in Figure 5 with the original solution proposed by Ahmad (1985). Since simulated Annealing is a stochastic procedure it is possible to rerun the problem with various initial seeds and thus obtain several competitive solutions to choose between.

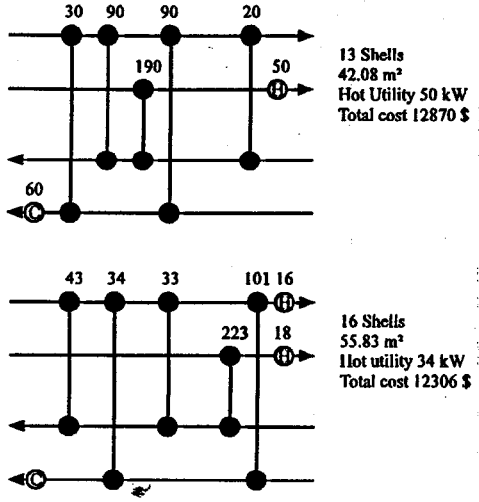


Figure 5. Example 1 design. Top Ahmad (1986), Bottom HEN Explorer (Nielsen, 1995)

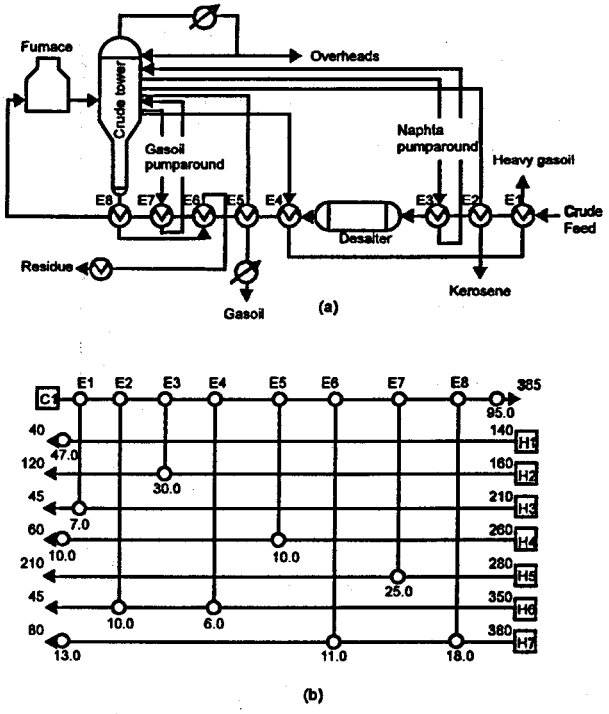


Figure 6. Example 2: Revamp of crude unit.

EXAMPLE 2

This example is taken from Shokoya and Kotjabasakis (1991) representing debottlenecking of a crude unit, where the task is to revamp the heat exchanger network for a 10% increase in throughput. A simplified flowsheet of the crude unit is given in Figure 6. The bottleneck of the plant is the capacity of the furnace. Presently the furnace can deliver 100 MW which is insufficient when the throughput is increased. Stream data and exchanger sizes are given in table 2 (increased flowrates in brackets).

Table 2 Streams	TS (°C)	TT (°C)	CP (kW/K)	h (kW/m²K)
C1	10 130 270	130 270 385	391.670 (430.837) 500.000 (550.000) 826.090 (908.699)	0.50 0.70 0.90
H1	140	40	470.000 (517.000)	0.20
H2	160	120	750.000 (825.000)	1.50
H3	210	45	42.420 (46.662)	0.80
H4	260	60	100.000 (110.000)	0.70
H5	280	210	357.140 (392.854)	1.0
H6	350 170	170 45	55.560 (61.116) 48.000 (52.800)	0.50 0.40
H7	380 160	160 80	145.460 (160.006) 125.000 (137.500)	0.40 0.30

Existing exchangers				
E1	255.0		E5	605.0
E2	595.0		E6	1288.0
E3	1744		E7	1733.0
E4	133		E8	1092.0

Table 2. Stream data and existing heat exchangers for example 2.

Shokoya and Kotjabasakis (1991) uses a so-called Area Matrix method based on pinch analysis to retrofit the heat exchanger network. Their result is compared with that obtained with HEN Explorer in Figure 7. The comparison clearly show that HEN Explorer is able to find very competitive solutions. This result is especially due to the features of Simulated Annealing algorithm which allow for a true simultaneous handling of all important trade-offs (energy, capital, units, etc.).

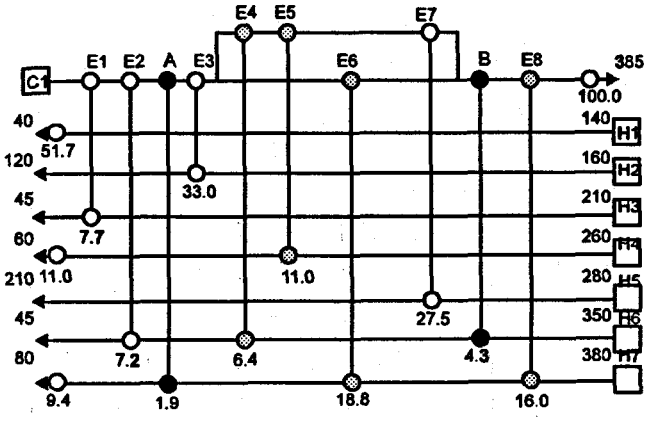
Algorithm efficiency

It should be kept in mind that the results presented here are compared with results obtained by manual methods. It therefore should be expected that automatic procedures will improve the results. So far, however, there have been no systematic attempts to solve the more detailed industrial HEN synthesis problem as stated in this presentation. This is because standard deterministic procedures in general will be unable to handle the complexity in the abovementioned problem.

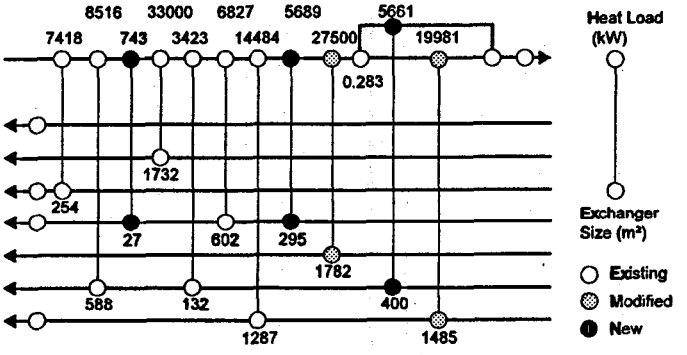
There is a price to pay for using a Simulated Annealing algorithm - Computational expense. From an industrial point of view this is only a problem if calculations last days. This can be the case if near optimum solutions are required for large scale problems with detailed modelling. In this case it can be desirable to combine deterministic methods (e.g. MILP or MINLP) using simple models with stochastic optimisation as implemented in HEN Explorer with full modelling. A general approach for combining these techniques has been proposed by Nielsen et al (1994).

Conclusion

A new framework for addressing the industrial HEN synthesis problem is presented. With the new framework it is possible to eliminate many of the simplifications that so far has been a limiting factor for widespread industrial use of HEN synthesis methods. To solve the complex problem that arises from the extended formulation a Simulated Annealing algorithm is used. The proposed methodology is implemented in the software tool HEN Explorer which has been successfully tested against several literature problems, and successfully applied on several industrial cases.



(A) Shokoya and Kotjabasakis (1991): Retrofit cost 364 k$



(B) HEN Explorer (Nielsen 1995): Retrofit cost: 320 k$

Figure 7. Example 2 designs.

References

Ahmad S., Heat Exchanger Networks: Cost Trade-Offs in Energy and Capital, *Ph.D. Thesis*, UMIST, Manchester, UK (1985).

Ahmad S., B. Linnhoff and R. Smith, Cost Optimum Heat Exchanger Networks-2. Targets and Design for Detailed Capital Cost Models, *Comput. chem. Engng*, **14**, p. 751 (1990).

Dolan W.B., P.T. Cummings and M.D. Le Van, Process Optimisation via Simulated Annealing: Application to Network Design. *AIChE Jl* **35**, p. 725 (1989).

Dolan W.B., P.T. Cummings and M.D. Le Van, Algorithmic Efficiency of Simulated Annealing for Heat Exchanger Network Design. *Comput. chem. Engng* **14**, p. 1039 (1990).

Floudas C.A., A.R. Ciric and I.E. Grossmann, Automatic Synthesis of Optimum Heat Exchanger Network Configurations. *AIChE Jl.*, **32**, p. 276 (1986).

Grossmann I.E., Mathematical Methods for Heat Exchanger Network Synthesis, *IEA Workshop on Process Integration - International Experiences and Future Opportunities*, Göteborg, Sweden (1993).

Grossmann I.E. and Z. Kravanja, Mixed-Integer Nonlinear Programming Techniques for Process Systems Engineering, *Computers chem Engng* **19**, p. S189 (1995).

Kirkpatrick S.C., C. Gelatt and M. Vecchi, Optimisation by Simulated Annealing, *Science* **220**, p. 671 (1983).

Nielsen J.S., V. Briones-Vallejo and A.C. Kokossis, An Integrated Framework for the Optimal Design of Heat Recovery Systems, Paper presented at *AIChE Annual Meeting, San Francisco, November* (1994).

Nielsen J.S., Energy Optimisation of Integrated Process Plants, *Ph.D. Thesis*, Technical University of Denmark, Lyngby, Denmark (1995).

Shokoya C.G. and E. Kotjbasakis, A New Targeting Procedure for the Retrofit of Heat Exchanger Networks, *The International Conference, Athens, Greece,* (1991).