Department of Energy Technology

Multiobjective Heat Exchanger Network Synthesis Based on Grouping of Process Streams

Timo P. Laukkanen

Aalto University

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Abstract

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Abstract

Heat exchanger network synthesis (HENS) is an important process synthesis problem and different tools and methods have been presented to solve this synthesis problem. This is mainly due to its importance in achieving energy savings in industrial processes in a cost-efficient way. The problem is also hard to solve and has been proven NP-hard (Nondeterministic Polynomial-time) and hence it is not known if a computationally efficient (polynomial) algorithm to solve the problem exists. Thus methods that provide good approximate solutions with reasonable computational requirements are useful. The objective of this thesis is to present new HENS approaches that are able to generate good solutions for HENS problems in a computationally efficient way so that all the objectives of HENS are optimized simultaneously. The main approach in accomplishing this objective is by grouping process streams. This is done either on the basis of the fact that in reality the process streams belong to a specific group or these groups are artificially developed. In the latter approach the idea is to decompose the set of binary variables i.e., the variables that define the existence of heat exchanger matches, into two separate problems. In this way the number of different options to connect the streams decreases compared to the situation where no decomposition is present. This causes the solution time to decrease and provides options for solving larger HENS problems. In this work the multiobjective HENS problem is solved either with the traditional weighting method or with an interactive multiobjective optimization method. In the weighting method the weights are the annual costs of the different objectives. In the interactive multiobjective optimization method the Decision Maker (DM) controls the decision-making process by classifying the objectives at each iteration. This multiobjective approach provides the benefit of using interactive multiobjective optimization, so that it is possible to find the solution that best satisfies the DM without too cognitive or computational load, and compared to the traditional approach of using fixed weights for the objectives, all the possible Pareto optimal solutions can be found. Overall the key value of this work is in presenting ways of simplifying a HENS problem.

Keywords Heat exchanger networks, Bilevel optimization, Interactive, Energy efficient

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Tiivistelmä

Tekijä
Timo Laukkanen

Väitöskirjan nimi
Lämmönsiirtoverkkojen synteesi virtojen ryhmittelyyn perustuvalla monitavoiteoptimoinnilla

Julkaisija Insinööritieteiden korkeakoulu

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Tiivistelmä
Lämmönsiirtoverkkojen synteesi on tärkeä prosessisynteesiongelma, koska tehokkaiden lämmönsiirtoverkkojen avulla prosessiteollisuudessa voidaan energiaa säästää kustannustehokkaasti. Lämmönsiirtoverkkojen synteesiongelma on vaikea ratkaista ja sen on todettu kuuluvan ei-polynomisten ongelmien luokkaan, joten sille ei todennäköisesti löydy yleistä polynomisesti konvergoituvaa ratkaisumenetelmää. Täten ongelman ratkaisemiseksi on hyödyllistä kehittää laskennallisesti tehokkaita approksimaatiomenetelmiä. Tämän työn tarkoituksena on kehittää laskennallisesti tehokkaita uusia lämmönsiirtoverkkojen synteesimenetelmiä, joiden avulla kaikkia ongelmassa olevia tavoitteita voidaan samanaikaisesti optimoida. Keskeisenä lähestymistapana tavoitteen saavuttamiseksi on prosessivirtojen ryhmittely. Ryhmittely perustuu joko siihen, että prosessivirrat kuuluvat tyypillisesti tiettyyn osaan prosessia tai ryhmittely suoritetaan keinotekoisesti. Keinotekoisessa ryhmittelyssä ajatuksena on hajottaa lämmönsiirtimien olemassaoloa kuvaavien binäärimuuttujien joukko kahteen osaan, jolloin eri prosessivirtojen välillä olevien mahdollisten kytkentöjen lukumäärä pienenee ja täten useimmissa tapauksissa myös synteesiongelman ratkaisemiseen käytetty aika pienenee mahdollistaen useampivirtaisten lämmönsiirtoverkkojen ratkaisemisen. Tässä työssä menetelmästä riippuen monitavoitteinen synteesiongelma ratkaistaan joko perinteisellä painokerroinmenetelmällä, jossa eri tavoitteita painotetaan niiden annualisoiduilla vuosikustannuksilla ja näiden vuosikustannusten summaa minimoidaan tai interaktiivisella monitavoiteoptimointimenetelmällä, jossa päätöksentekijä hallitsee päätöksentekoprosessia luokittelemalla tavoitteita kullakin iteraatiokierroksella. Interaktiivisen monitavoiteoptimointimenetelmän etuna on, että kaikki mahdolliset Pareto-optimaaliset ratkaisut voidaan löytää ilman liian suurta kognitiivista ja laskennallista kuormitusta. Työn päätuloksena on joukko menetelmiä, joiden avulla lämmönsiirtoverkkojen synteesiongelmaa voidaan yksinkertaistaa, jolloin ongelma voidaan tehokkaasti ratkaista.

Avainsanat Lämmönsiirtoverkko, Kaksitaso-optimointi, Ineraktiivinen, Energiatehokkuus,

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Preface

".. one who is searching for something does not travel very fast."
The telephone repairman in E. B. White's storybook Stuart Little

I have had a great opportunity to do research in an interesting and challenging topic. Although working on this thesis has been a long journey, I have enjoyed almost all moments of it.

I want to thank my supervisor, emeritus professor Carl-Johan Fogelholm, for the encouraging comments and opportunity to work on this thesis in an inspiring atmosphere. The contribution of my instructor, Dr. Tor-Martin Tveit, in participating in the writing in some of the articles and commenting all of the work in this thesis is indispensable. I also want to thank professor Kaisa Miettinen and researcher Vesa Ojalehto for their central contribution in some of the articles of this thesis and for guiding me to the very interesting world of multiobjective optimization. I thank PhD Jussi Manninen and professor Mika Järvinen for commenting this thesis in a very limited time-frame.

From our research group I want to thank all current and former workers for an inspiring and enjoyable working atmosphere and for good times both in and out of office.

Many Finnish companies and associations have effected and financed my work either directly or indirectly. For this I am very thankful.

Without my family this journey would have been much tougher to make. Marjukka, Minea and Frida, I thank you that in my life there is so much more than just research work.

Espoo, May 23, 2012,

Timo P. Laukkanen

Contents

List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I Laukkanen, T., Tveit, T.-M. and Fogelholm, C.-J.. Simultaneous heat exchanger network synthesis for direct and indirect heat transfer inside and between processes. *Chemical Engineering Research and Design*, In Press, Corrected Proof, Available online 22 December 2011.

II Laukkanen, T. and Fogelholm, C.-J.. Heat exchanger network synthesis- A bilevel decomposition method based on stream data grouping. In *CHEMICAL ENGINEERING TRANSACTIONS, Volume 12, pages 333-338, 2007, Edited by Jiri Klemes, 10th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction*, Ischia, Naples, Italy, 24-27 June 2007.

III Laukkanen, T. and Fogelholm, C.-J.. A bilevel optimization method for simultaneous synthesis of medium-scale heat exchanger networks based on grouping of process streams. *Computers & Chemical Engineering*, 35, 2389-2400 2011.

IV Laukkanen, T. and Tveit, T.-M. and Ojalehto, V. and Miettinen, K. and Fogelholm, C.-J.. An interactive multi-objective approach to heat exchanger network synthesis. *Computers & Chemical Engineering*, 34, 943-952 2010.

V Laukkanen, T., Tveit, T.-M., Ojalehto, V., Miettinen, K., and Fogelholm, C.-J.. Bilevel heat exchanger network synthesis with an interactive multi-objective optimization method. *Applied Thermal Engineering*, In Press, Uncorrected Proof, Available online 8 May 2012.

VI Nykopp, J., Laukkanen, T., Tveit, T.-M., and Fogelholm, C.-J.. A tool for automatic heat flow grid visualisation for heat exchanger networks developed using the SYNHEAT model. In *Proceedings of the 18th International Congress of Chemical and Process Engineering CHISA 2008, Czech Society of Chemical Engineering*, Prague, Czech Republic, 24-28 August 2008.

Author's Contribution

Publication I: "Simultaneous heat exchanger network synthesis for direct and indirect heat transfer inside and between processes"

Publication I presents a MINLP model for HENS that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes. The indirect heat transfer is accomplished by using intermediate streams. Intermediate streams are used in order to reduce the number of transfer units between processes, because of the physical distance between the processes and for operational flexibility reasons. The main objective of the model is to provide a new HENS model that is specially directed to situations where a process plant is divided into specific processes. In this case the streams are grouped according to the topological fact that different streams exist in different processes. The weighting method using fixed weights (annual costs) is the multiobjective approach used to solve the problem. Publication I shows that considering the possibility of using intermediate streams for indirect heat transfer can sometimes be beneficial, especially if direct heat transfer between streams in different processes is restricted or forbidden. The author developed the model, calculated the results, and wrote the article. The co-authors contributed by commenting the work.

Publication II: "Heat exchanger network synthesis- A bilevel decomposition method based on stream data grouping"

Publication II presents a simultaneous HENS method that uses bilevel optimization, stream data grouping, and the aggregation of streams. The objective of the method is to generate good solutions for HENS in a computationally efficient way so that all the objectives of HENS are optimized simultaneously. The models of the method are based on the Synheat superstructure. The idea of the method is to decompose the set of binary variables, i.e., the variables that define the existence of heat exchanger matches, into two separate problems. In this way the number of different options to connect the streams decreases compared to the situation where no decomposition is present. The difference compared to Publication III is that in Publication II the aggregate streams are developed from all the hot or cold streams that are not present in a specific group. The weighting method with fixed weights is the multiobjective approach used, so the overall objective is to minimize the total annual cost of the heat exchanger network. The results obtained by solving examples from the literature with the method show that the method can give comparable results for HENS problems with reduced computational effort. The author developed the method, calculated the results, and wrote the article. The co-author contributed by commenting on the work.

Publication III: "A bilevel optimization method for simultaneous synthesis of medium-scale heat exchanger networks based on grouping of process streams"

Publication III presents a simultaneous HENS method that uses bilevel optimization, stream data grouping, and the aggregation of streams. It is an improved version of Publication II. Both have the same basic idea and objectives. The difference compared to Publication II is that in Publication III the aggregate streams are developed from all the hot or cold streams present in a specific group. Some developments are also made in the steps of the method. The author developed the method, calculated the results and wrote the article. The co-author contributed by commenting on the work.

Publication IV: "An interactive multi-objective approach to heat exchanger network synthesis"

Publication IV presents an interactive multiobjective approach to HENS in which an implementation of the interactive multiobjective optimization method NIMBUS, called IND-NIMBUS, is integrated with the GAMS modeling system. This enables GAMS to be used for solving multiobjective optimization problems without using weighting factors. The Synheat model is used as a superstructure generating model for HENS and no stream grouping is used. In the integration of GAMS and IND-NIMBUS a simplified implementation of the NIMBUS method is applied and the tool is called the A–GAMS–NIMBUS-tool. Previously, interactive multiobjective optimization has not been applied to HENS problems. With interactive multiobjective optimization there is a possibility of finding the network that best satisfies the Decision Maker without too great a cognitive or computational load, and compared to the traditional approach of using fixed weights for the objectives, all the possible (local) Pareto optimal solutions can be found. The results obtained by solving examples from the literature with the method show that the method can give comparable results for HENS problems. The author developed the integration of IND-NIMBUS and GAMS with the aid of co-author Vesa Ojalehto, calculated the results, and participated in writing the article. The co-authors participated in developing the original idea, in writing the article, and in commenting on the work. It is important to remark that one of the co-authors, Kaisa Miettinen, is the developer of the NIMBUS multiobjective optimization method.

Publication V: "Bilevel heat exchanger network synthesis with an interactive multi-objective optimization method"

Publication V integrates the methods presented in Publication III and Publication IV, thus combining two innovative methods and providing a means to solve HENS problems in a computationally efficient way and so that all the Pareto optimal solutions can be found. The results obtained by solving examples from the literature with the method show that the method can give competitive results for HENS problems. The author developed the integration of the methods, calculated the results, and partly wrote the article. The co-authors participated in writing the article and commenting on the work.

Publication VI: “A tool for automatic heat flow grid visualisation for heat exchanger networks developed using the SYNHEAT model”

Publication VI introduces HeVi, a new visualization tool for heat exchanger networks that are optimized using the Synheat superstructure. HeVi is a combination of a sankey-diagram and a stream grid. The author proposed the need for the tool, created the specs for the program, tested the program, and participated in writing the article. The co-author J. Nykopp coded the program and participated in writing the article. The co-author T.-M. Tveit commented and participated in writing the article. Co-author C.-J. Fogelholm commented on the work and proposed the idea of also presenting the network as a sankey-diagram.

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List of Tables

Nomenclature

ΔT_{min}	minimum temperature difference between two streams exchanging heat
A–GAMS–NIMBUS	HENS method in Publication IV
CC	Composite Curve
CU	Cold Utility
G	Groups
GA	Genetic algorithm
GAMS	General Algebraic Modeling System
GCC	Grand Composite Curve
HEN	Heat Exchanger Network
HENS	Heat Exchanger Network Synthesis
HeVi	A visualization tool of optimized HENs in Publication VI
HRAT	Heat recovery approach temperature
HU	Hot Utility
IND-NIMBUS	Interface to the NIMBUS method
Indirect	MINLP model in Publication I
LP	Linear Programming
MINLP	Mixed Integer Non-linear Programming
MoBilevel1	HENS method in Publication V

NIMBUS	Interactive multiobjective optimization method
NLP	NonLinear Programming
NP	Nondeterministic Polynomial-time
PA	Pinch Analysis
PDM	Pinch Design Method
PNS	Process Network Synthesis
SA	Simulated annealing algorithm
SingBilevel1	HENS method in Publication II
SingBilevel2	HENS method in Publication III
Synheat	Synheat model
TS	Tabu search algorithm

1. Introduction

1.1 Background

Industry is one of the main consumers of energy in modern societies. For example, in Finland, industry consumed 50% (550396 TJ) of final energy consumption (1110030 TJ) in 2008 (Finland [27]). Partly for this reason, industry also produced 30.6% (excluding public energy conversion) of Finland's CO_2 emissions in 2008 (Finland [28]). Hence increasing energy efficiency, and thus increasing primary energy savings and reducing emissions in industry, is an necessary objective for making industrial societies sustainable. Sustainability also includes economic sustainability, so energy savings and CO_2 emission savings should be carried out in a way that does not harm the competitiveness of industry.

Increased energy efficiency is one of the major options for reducing energy consumption in industry and hence reducing emissions. In the EU the energy-saving potential in industry is assumed to be 25% from 2005 to 2020 (of the European Communities [68]). One possibility for energy savings in industry is to enhance heat recovery so that fuel consumption can be reduced or electricity production increased or both. One option for cost-effective heat recovery is with effective and optimized heat exchanger networks and for this reason Heat Exchanger Network Synthesis (HENS) has been an active research area in recent decades. Additional academic interest results from the fact that the problem is hard to solve. As Furman and Sahinidis [34] proved, the problem is NP-hard (Nondeterministic Polynomial-time) and hence it is not known if a computationally efficient (polynomial-time) algorithm to solve the problem exists. One dimension of NP-hardness in HENS is that increasing the number of possible heat exchanger matches (increasing the number of streams) increases the number of possible heat exchanger structures exponentially. Thus methods

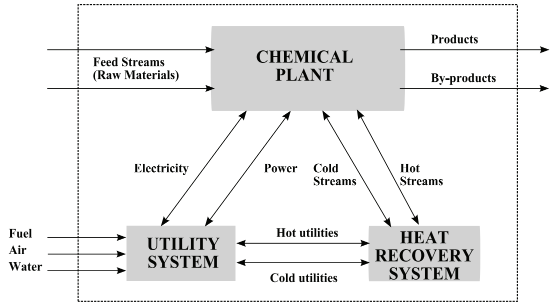

Figure 1.1. An overall process system.

that provide good approximate solutions with reasonable computational requirements are vital. Sometimes these methods can be generalized and applied to other process systems engineering problems as well. The effectiveness of HENS methods is also important for the reason that HENS is typically only one subproblem in designing a process (i.e., process synthesis) and many different process configurations need optimized heat exchanger networks. This means that many different heat exchanger networks have to be obtained with varying data, emphasizing the need for HENS methods that provide robustly good results fast.

Figure 1.1 (adopted from Floudas [29]) shows how an industrial process system consists of a chemical plant, an utility system, and a heat recovery system, and how these subsystems interact with each other.

1.2 Research problem

The objective for most of the research done on heat exchanger network synthesis problems can be formulated as follows: *The objective is to design a heat exchanger network that minimizes the total annualized cost, given sets of hot streams, cold streams, hot utilities, and cold utilities. Each hot and cold stream has a specific heat capacity flow rate and a start and target temperature.*

In this work a slightly changed formulation is used:

The objective is to design a heat exchanger network that simultaneously optimizes the required utility consumption, number of heat exchanger units and the *heat transfer area or the weighted sum of the cost of these objectives, given sets of hot streams, cold streams, hot utilities and cold utilities. Each hot and cold stream has a specific heat capacity flowrate, a start- and target temperature.*

The key research question in this work is how can the objective defined above be reached so that compared to existing methods the computational effort is decreased without loosing the quality of the results and how can multiobjective optimization be used in reaching this objective.

1.3 Objective of the thesis

The objective of this thesis is to develop new HENS approaches that are able to generate good solutions in a computationally efficient way so that all the objectives of the synthesis problem are optimized simultaneously. The main approach used in accomplishing this objective is process stream grouping. Either this grouping is based on the fact that in reality the process streams belong to a specific process or these groups are artificially developed. In the latter approach the idea is to decompose the set of binary variables, i.e., the variables that define the existence of heat exchanger matches, into two separate problems. In this way the number of different options to connect the streams decreases compared to the situation where no decomposition is present. This causes the solution time to decrease, at least in most cases, and provides options for solving larger HENS problems. This approach is the key innovation of this work. In other words, the key value of this work lies in presenting a good way of simplifying a HENS problem so that HENS problems can be solved efficiently while at the same time good results are obtained.

The HENS problem is solved with two different multiobjective approaches. The first approach uses the traditional weighting method where the (fixed) weights are the annual costs of the different objectives, i.e., hot utility consumption, cold utility consumption, the number of heat exchangers, and the heat transfer area, and the weighted sum of the objectives is minimized. In this way the multiobjective optimization problem is transformed or scalarized into a single-objective optimization problem. The clear benefit of the weighting method is that most HENS solutions are obtained with it, so new results can be compared with existing ones. The problem with this approach is that if the problem is non-convex and

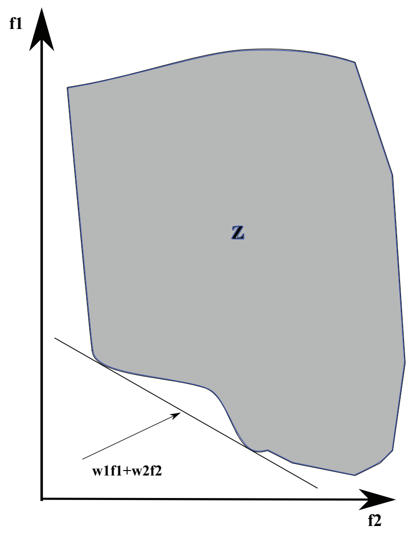

Figure 1.2. Weighting method for a nonconvex optimization problem.

linear weights are used, not all the Pareto optimal solutions can be found, as shown in Figure 1.2, where the Pareto optimal solutions in the middle part of the Pareto front are not found. This non-convex behavior was also shown to happen in HENS by Björk and Westerlund [10]. The second multiobjective approach utilizes an interactive multiobjective optimization method in which the Decision Maker (DM) controls the decision-making process by classifying the objectives at each iteration. With this approach, all the Pareto optimal solutions can be found.

1.4 Scope of the thesis

In this work the focus is on solving the general HENS problem described in Section 1.2. The methods presented are aimed at solving the greenfield design problem, i.e. a new design problem, although after modifications they could be applied to retrofit situations as well.

The methods presented in this work use the same HENS assumptions that are typical for most of the HENS methods. These assumptions are:

- fixed specific heat capacity of streams;

- no consideration of pressure drops in heat exchangers or pipes;
- fixed inlet and outlet temperatures of streams;
- fixed heat transfer coefficients;
- countercurrent heat exchangers.

1.5 Challenges in HENS

Although a lot of different methods for HENS have been presented, a number of major challenges still remain to be solved. Typically, newly introduced HENS methods can improve or solve one or two of the challenges but at the same time at least one of the challenges is impaired. The major challenges in HENS are listed below.

- Combinatorics. Combinatorics arises from the fact that increasing the number of possible heat exchanger matches increases the number of possible heat exchanger structures exponentially ($2^{possible\ matches}$). In principle the solution time increases exponentially with the increasing possible number of heat exchanger matches. Combinatorics can also be a problem if the solution region is systematically divided into subsections (for example, in order to find the globally optimum solution). Combinatorics is a particular problem for larger problems with tens of process streams.

- Local solutions. Local solutions arise for the reason that if some kind of problem decomposition is applied or algorithms that can guarantee only locally optimal solutions are used and the solution space is non-convex, it is not possible to guarantee that the final solution is also globally optimal. Good solutions can be reached, but this depends on the starting solution. The major problem with local solutions is that typically there is no knowledge of how far the local solution is from the global solution, thus creating a lack of confidence in the results. With deterministic solvers that guarantee globally optimal solutions the problem of local solutions can be avoided, but then as a result of combinatorics only small-sized problems can be solved. Deterministic algorithms are algo-

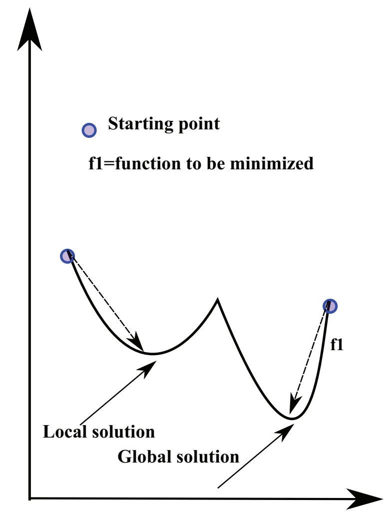

Figure 1.3. The effect of a starting point on the final solution while using local solvers.

rithms that behave predictably and, with a particular input, will always produce the same output. With increasing computer capacity, steadily bigger and bigger problems can be solved to global optima, but without fundamental improvements in optimization algorithms, this progress is very slow. Figure 1.3 shows how the solution of an optimization problem depends on the starting solution if local solvers are used.

- Flexibility. In real industrial processes operational flexibility is a key factor. The processes should also operate efficiently when processes or subprocesses are not operating at full capacity or when process parameters vary, for example, because of changes in the outside environment and during startups and shutdowns. With increased heat integration this flexibility decreases. This is a particular problem if processes that are heat-integrated with each other are owned by different companies. In principle this decrease in flexibility can be solved with utility exchangers that are big enough to heat or cool every process stream to its target temperature. It can be assumed that this approach is not the most cost-efficient one.

- Model simplifications. Most HENS approaches use some kinds of simplifications in order to make the problem solvable. These simplifications occur in basic assumptions, such as that the heat capacity flow rate of a process stream is constant and heat transfer coefficients of process streams are constant, in model formulations such as in assuming the isothermal mixing of split process streams in some superstructures, and in algorithms, such as decomposing the problem by solving the different objectives sequentially. This is a necessity, but these simplifications can cut off the best solutions, so these simplifications should be challenged and other simplifications that are not so harmful should be used.

- Integration with other process synthesis problems. As mentioned, HENS is just one step in designing a process. Typically, before HENS the basic structure of the process has already been decided and most major process units have been designed. In this way the basic design parameters (e.g., the process stream mass flow rate and start and target temperatures) of heat exchanger networks have already been fixed. It would probably be beneficial regarding the overall process synthesis if these parameters could be systematically challenged prior to HENS while taking into account the effects of heat exchanger networks. In this way the number of different HENS calculations would decrease and better processes would be obtained.

Because of the challenges mentioned above, the heat exchanger network synthesis problem still remains a problem needing additional research and improvement. The challenges that the methods developed in this thesis focus on are model simplifications and combinatorics.

1.6 Outline of the thesis

This thesis consists of six original research articles and a summary of the research. Figure 1.4 shows how the six publications are connected to each other. The first, Publication I, presents a heat exchanger network synthesis MINLP model that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes. The abbreviation for the model used in this thesis is *Indirect* and it is based on the stage-wise superstructure called Synheat (Yee and Grossmann [89]), as are all the HENS models in

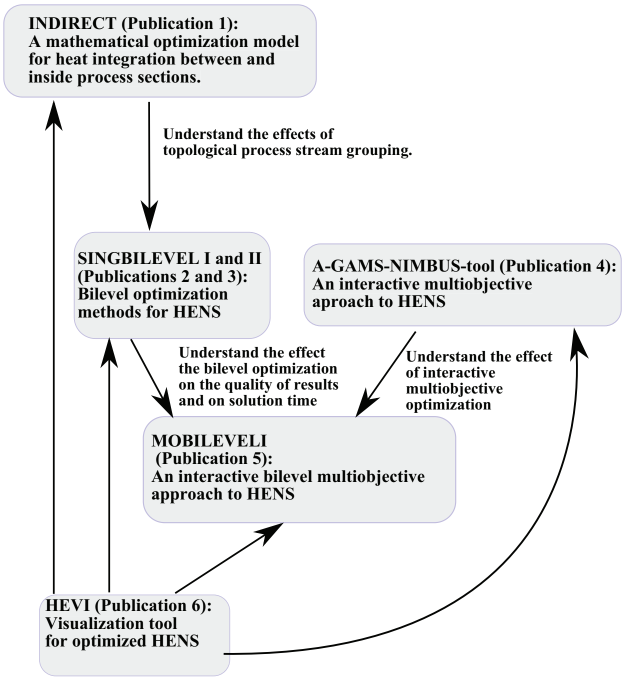

Figure 1.4. The connections between the publications.

this thesis. The main objective of this publication is to study the effects of heat integration when the streams have specific groups which they belong to, but the objective is not to make the solution procedure more efficient. The weighted sum of the functions that are minimized is the multiobjective approach used in the model.

One of the results obtained with the *Indirect* model is that heat integration between streams in different process groups can be beneficial in some situations. Another result partly obtained from the *Indirect* model and partly from the literature is that the computation time of simultaneous HENS models models restricts the size of solvable HENS problems. The objective of Publication II (abbreviation *SingBilevelI*) and Publication III (abbreviation *SingBilevelII*) is to solve a general simultaneous (where all the objectives are optimized at the same time) HENS problem so that the computation time is also taken into account without the quality of the solutions being harmed. In these articles process streams are forced into groups. In Publication III hot and cold aggregate streams for each group are formed from each group's hot and cold process streams. In Publication II aggregate streams are built from streams that are not present in that group. Next, the total annual cost of the heat exchanger network is minimized, but in such a way that direct heat exchanging between streams in different groups is not allowed. This means that the hot streams of a specific group can exchange heat only with the cold streams in the same group and with the cold aggregate streams of other groups. Hence direct heat exchanging between streams in different groups is not allowed. Process streams and aggregate streams can also exchange heat with utility streams. In the final step, all the streams are allowed to exchange heat with each other, but in such a way that the binary variables indicating the existence of heat exchanging matches between streams in the same group are fixed according to the results obtained from the previous step. In order to get a good solution, the last two steps are solved repeatedly with integer cuts added to matches that indicate the existence of heat exchange between streams in the same group. The models of the method are based on the Synheat superstructure approach presented by Yee and Grossmann [89]. The weighted sum of the functions that are minimized is the multiobjective approach used in the methods.

Although the calculation time of simultaneous HENS can be reduced with the methods presented in Publication II and Publication III, there is the problem that that when the approach of the weighted sum of the functions that are minimized is used, some interesting solutions can be cut off, especially when the costs of different objectives are uncertain and need to be varied. To solve this problem, Publication IV presents an interactive multiobjective method for simultaneous HENS. The abbreviation for the method used in this thesis is the *A–GAMS–NIMBUS-tool*. In the method an implementation of NIMBUS, called IND-NIMBUS, is integrated with the GAMS modeling system. The interactive approach was chosen as the multiobjective approach, because then the designer of the network is in charge of the network design procedure and the calculation time does not increase too much compared to other multiobjective approaches.

In order to combine the reduced calculation effort with the interactive multiobjective optimization approach, Publication V, is presented. This article combines the methods developed in articles Publication III) and (Publication IV into a bilevel, simultaneous, and interactive HENS method. The abbreviation for the method used in this thesis is *MO-BilevelI*.

Publication VI presents *HeVi*, a visualization tool for an automatic heat flow grid of optimized HENs that are based on the Synheat model. *HeVi* is a combination of a Sankey diagram and a stream grid. *HeVi* is used to visualize the networks in all the other publications of this thesis thus aiding the designer of the networks in her/his aim of developing good networks.

In the overview part of this thesis, Chapter 2 presents the previous key developments of the HENS methods and how these relate to the methods and models presented in this thesis. In Chapter 3 the different HENS methods developed in this thesis are presented. In Chapter 4 the major results of examples solved with the methods presented here are introduced. In Chapter 5 the main conclusions of this thesis, together with a discussion of the contribution of this work, are presented. A discussion of possible future work is also given.

2. Heat exchanger network synthesis

In this chapter a review of the most important contributions to Heat Exchanger Network Synthesis (HENS), especially in relation to this thesis, is presented.

HENS has been an active research area for more than 40 years. This is mainly due to its importance in achieving energy savings in industrial processes in a cost-efficient way. The problem is also hard to solve and Furman and Sahinidis [34] proved that the problem is NP-hard and hence it is not known if a computationally efficient (polynomial) algorithm to solve the problem exists. Thus methods that provide good approximate solutions with reasonable computational requirements are useful. A lot of different tools and methods have been presented to solve the HENS problem. Extensive reviews of these methods can be found in Gundersen and Naess [38] and Furman and Sahinidis [35]. Recently Morar and Agachi [65] performed a comprehensive review of the major turning points and emerging trends in the development and improvement of heat integration and HENS methods through the years 1975-2008.

2.1 Basic heat exchanger network synthesis

Most of the HENS methods that have been developed try to solve the general problem defined in Section 1.2 and can be classified as either thermodynamic synthesis methods, deterministic mathematical programming synthesis methods or stochastic synthesis methods, although in many of the methods parts or ideas of other methods of other types are used. Another classification is sequential synthesis versus simultaneous synthesis methods. Sometimes the simultaneous methods utilize some kind of targeting tool adapted from sequential methods in order to reduce the solution space.

2.1.1 Thermodynamic synthesis methods

In the group of thermodynamic optimization methods, the Pinch Design Method (PDM) (see, for instance, Linnhoff and Hindmarsh [57], Linnhoff [54], Linnhoff [55]) is probably the most famous and most used HENS method, and it is also widely used in industry. PDM is a sequential synthesis method. The basic idea in the sequential synthesis strategy is to decompose the problem into subproblems. Prior to this decomposition the temperature range of the process streams is divided into intervals providing thermodynamically correct solutions. Also prior to the decomposition, the overall minimum temperature difference (called HRAT (Heat Recovery Approach Temperature) or ΔT_{min}) that both sides of a heat exchanger must have at the very least is decided. In most cases hot and cold utilities are minimized in the first subproblem. In the second subproblem the number of heat exchanger units is minimized, together with the fixed amount of utilities obtained from the previous subproblem. In the third and last subproblem the heat exchanger area is minimized with the fixed amount of utilities and number of heat exchanger units. After this the three subproblems are solved once again with a new value of HRAT. In PDM, the minimization of the utilities is the first sequential step and is called Pinch Analysis. In this analysis tool, Composite Curves (CC) and Grand Composite Curves (GCC) (see, for instance, Hohmann [43], Linnhoff et al. [58]), can be drawn with the knowledge of basic stream data and a given HRAT. Form these curves the pinch point and the values for minimum hot and cold utilities can be obtained. In Figure 2.1 examples of CC and GCC are shown. The pinch point is a temperature that divides the process into two areas, one with a heat deficit and one with a heat surplus. With this information heat exchanger networks can be designed following the three basic pinch rules:

- do not transfer heat across the pinch point;
- do not heat streams with hot utility below the pinch point;
- do not cool streams with cold utility above the pinch point.

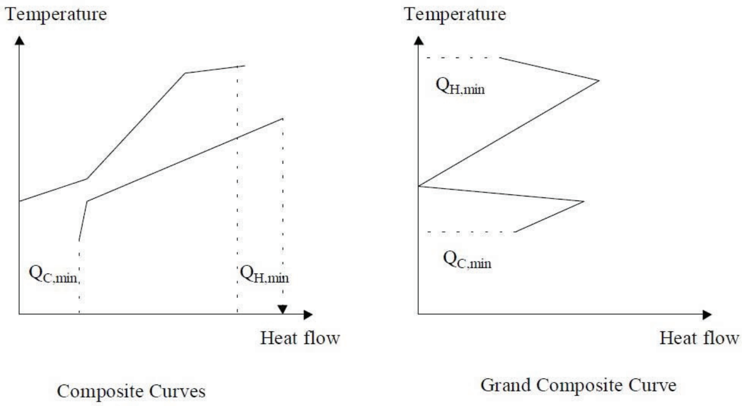

Figure 2.1. Pinch curves.

The sequential synthesis strategy is used to reduce the computational requirements of designing heat exchanger networks, but unfortunately there is no guarantee that globally optimal networks will be found with the sequential synthesis strategy or how far the solution found is from the global one and the overall procedure is still NP-hard. But the benefit of thermodynamic analysis tools such as PDM is that the designer of the network is in control of the design procedure.

2.1.2 Mathematical programming methods

Mathematical programming has also been used with the sequential approach to decompose the problems into sub-problems. The most widely used sequential method consists of three optimization models that are solved in a series, where the first model minimizes the utility cost (Cerda et al. [19], Papoulias and Grossmann [69]), the second model minimizes the number of units (Cerda and Westerberg [18]) and the third model minimizes the investment cost related to the size of the heat exchangers (Floudas et al. [32]). This leads to solving an optimization problem of the form:

$$\begin{aligned} &\min && (\text{cost of heat exchanger surface area}) \\ &\text{s.t} && \min\ (\text{number of units}) \\ & && \text{s.t.}\ \min\ (\text{utility consumption}). \end{aligned} \tag{2.1}$$

As can be seen from Equation 2.1 the typical order of importance of the different objectives assumed in the sequential methods is that utility consumption is the most important objective, followed by the number of units objective and heat transfer area objective. Pettersson [71] developed a computationally efficient sequential strategy in which the terms involved

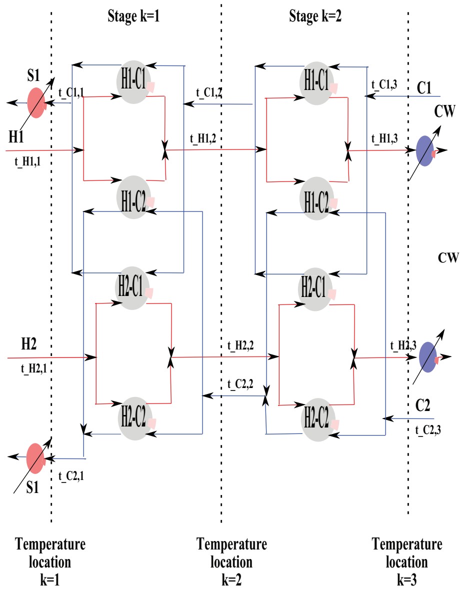

Figure 2.2. Synheat superstructure with two stages, two hot streams and two cold streams.

in the objective function are more accurate in each sequential step.

In order to take better account of the trade-offs of the different objectives in designing heat exchanger networks, several simultaneous methods have been developed, of which the Synheat model by Yee and Grossmann [89] is one. Synheat is based upon a stage-wise superstructure. An example of a stage-wise superstructure can be seen in Figure 2.2. The benefit of the Synheat model is that the dimensionality of the model is reduced and the set of constraints becomes linear, because an isothermal mixing assumption is used at the end of each stage and hence the only non-linearity and non-convexity is in the objective function. On the other hand this isothermal mixing assumption can cut off the globally optimal solution. Additionally, some structures are excluded from the superstructure as shown in Figure 2.3.

In this thesis the Synheat model is used as a base model for all HENS models, which are solved using deterministic optimization algorithms.

Another example of a simultaneous HENS method is the MINLP model by Ciric and Floudas [22], where the utility load is an explicit variable, heat is allowed to flow through the pinch point, and the optimal structure is selected from a hyperstructure containing all the alternative matches and network configurations. The problem with this approach is that even

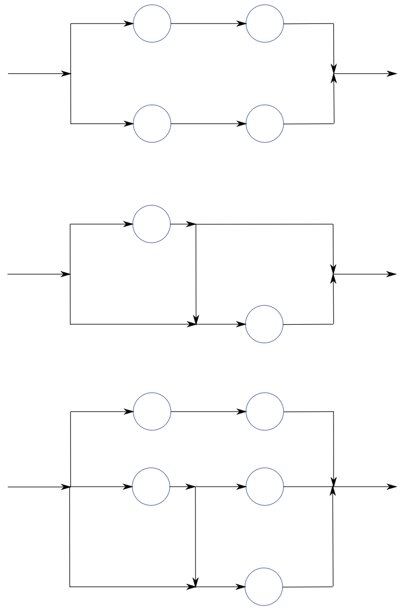

Figure 2.3. Structures excluded with the Synheat superstructure.

though the globally optimal solution can be found, at least with algorithms that are able to guarantee the global optimum, the computational requirements increase heavily compared to the Synheat-model. If algorithms that can guarantee only locally optimal solutions are used, finding good or even feasible solutions can be tedious because the number of non-convex equations increases.

Because the simultaneous HENS methods provide the possibility of finding the global optimal solution to the original HENS problem, it would be very beneficial to exploit this possibility by using algorithms that can guarantee the global optimum or to use convexification techniques that also provide the global optimum when algorithms providing only local solutions are used. Quesada and Grossmann [74] developed a rigorous global optimization algorithm for HENS with a fixed topology. Adjiman et al. [2] solved HENS problems with a global optimization algorithm using an assumption that areas have linear cost functions. On the basis of the Synheat model, Zamora and Grossmann [92] and Zamora and Grossmann [93] applied a branch and contract algorithm for global optimization of HENS. Björk and Westerlund [13] applied convexification techniques so that algorithms guaranteeing only locally optimal solutions can also be used to ensure the global optimum. The problem with global optimum algorithms and convexification techniques is that the solution times can become remarkably long, even in problems that have just a few process streams.

In this thesis only solvers that are able to provide local solutions for non-convex problems are used.

2.1.3 Stochastic synthesis

Stochastic methods based on the use of heuristic algorithms or evolutionary algorithms such as genetic algorithms (GA), simulated annealing algorithms (SA), and Tabu search algorithms (TS) have also been used in HENS. These HENS methods can in general be classified into the group of simultaneous synthesis methods, although typically these methods use some kind of targeting phase prior to their use or they are used as a solution method for a specific step of the sequential synthesis method. Grimes et al. [36] used an evolutionary algorithm to solve the minimum number of units step in the sequential synthesis method. Lewin et al. [52] used genetic algorithms to find out optimal HEN structures, together with a Linear Programming (LP) algorithm, in fixing the heat loads of units. In Lewin [51] the same procedure was used, but there a NonLinear Programming (NLP) algorithm was used together with the GA to fix the heat loads of the units. Recently, Khorasany and Fesanghary [46] used a similar hybrid approach, where the HEN structures are determined with a heuristic harmony search algorithm. Toffolo [85] used an unconstrained graph representations of a HEN that was solved with a GA to optimize the HEN structures and an NLP to manage the heat load distribution among the exchangers. Another hybrid approach was presented by Ravagnani et al. [76], where a pinch analysis technique was used together with a GA in HENS. Dipama et al. [24] presented a decomposition made at the pinch point that was used together with a GA for HENS without stream splitting. Wei et al. [87] used an algorithm they named GA/SA (parallel genetic/simulated annealing algorithm) with the Synheat model without the isothermal mixing assumption for simultaneous HENS. Lin and Miller [53] used a Tabu search algorithm. Recently X. Luo and Fieg [88] presented a hybrid algorithm where a GA was combined with other search strategies (simulated annealing, local optimizing strategy, structure control strategy etc.) to enhance the search. The method is based on the stage-wise superstructure of the Synheat model.

The benefit of these stochastic or heuristic methods is that no derivative information of functions is needed. The problem with stochastic or heuristic methods is that there is no guarantee that the global optimum has been found and it might take a very long time to get even decent HEN solutions. It can also be hard to set the correct parameters needed in the methods.

In this thesis all the methods are solved with deterministic algorithms.

2.1.4 Grouping of streams

Because HENS on a large scale (over 15 process streams) is a complex problem, grouping of process streams has been used to solve the problem. Fieg et al. [26] presented a HENS method, based on the stage-wise superstructure of the Synheat model, where first a hybrid GA is used to find functional groups (sub-networks), which are then optimized separately. A similar approach was presented by Björk and Pettersson [12] for greenfield HENS and Björk and Nordman [11] for retrofit HENS, where the development of groups was achieved with a GA and the groups (sub-networks) are solved separately with mathematical programming algorithms. A block decomposition approach, where the composite curves are decomposed into a number of blocks in which straight line segments approximate the composite curves giving quasi-composites, was presented by Zhu et al. [95]. Later Zhu [94] developed this concept into an automated HENS method.

In this thesis too the grouping of process streams is used in HENS. In this work process streams are grouped either according to topological reasons, *i.e.*, process streams are part of a specific process sections (Indirect model) or are artificially developed (SingBilevelI, SingBilevelII, and MOBilevelI). Compared to the other methods where the grouping of process streams is applied, in this thesis heat can be transferred between streams in different groups. This is achieved with aggregate streams that represent the process streams of other groups. This possibility, according to the results of the examples solved, is not that harmful for the quality of the optimized network.

2.1.5 Multiobjective methods

In the formulation presented in Chapter 1.2 the multiobjective nature of the heat exchanger network synthesis problem has been transformed into a single-objective problem using annualized cost. This is done although the true nature of the problem can be better captured by formulating several individual objectives in the modeling phase instead of only one. The resulting problem with conflicting objectives can then be solved by using multiobjective optimization methods (see, e.g., Miettinen [59]). Multiobjective optimization enables the interdependencies between the conflicting objectives to be considered and in that way one can learn about the problem being considered. On the other hand, it is not necessary to estimate the annualized cost of individual objectives.

Chen and Hung [20] developed a multiobjective mixed integer linear programming model for flexible heat exchanger network synthesis, that simultaneously considers minimum utility consumption, maximum source-stream temperature flexibility, and the minimum number of matches. They applied a fuzzy multi-objective decision-making method to deal with the objectives of their model. Agarwal and Gupta [3] used a genetic algorithm to generate a set of solutions approximating the Pareto optimal solutions of heat exchanger network synthesis problems. All of the multiobjective HENS research work described above uses *a posteriori* methods, where the DM is presented with a set of Pareto optimal solutions after its generation. For a heat exchanger network synthesis problem this generation is computationally expensive and the DM has to select one solution from a very large set of solutions, which can be cognitively very demanding.

In this thesis two multiobjective optimization approaches are used. The first one is the traditional approach of minimizing the weighted sum of the functions that are minimized. This approach leads to optimizing a single objective and for this reason is not necessarily even considered as a multiobjective approach, even though multiple objectives are optimized. The other multiobjective approach used is interactive multiobjective optimization. Interactive multiobjective optimization has not previously been used in HENS.

2.2 Extensions to basic heat exchanger network synthesis

For the basic heat exchanger network problem a lot of different extensions have been introduced. In the majority of these extensions the aim is either to describe the problem in more detail, or to integrate HENS into other process synthesis problems.

One natural extension is the consideration of retrofit situations, although retrofit situations can equally well be considered as belonging among the basic HENS problems. Here retrofit situations are considered as extensions of basic HENS approaches, because additional data is needed. Retrofit methods based on pinch concepts include those proposed by Tjoe and Linnhoff [84], Polley et al. [73], Shokoya and Kotjabasakis [80], and Carlsson et al. [17]. Mathematical programming methods include those of Ciric and Floudas [21], Yee et al. [90], Asante and Zhu [6], Asante and Zhu [7], Briones and Kokossis [15], and recently, Sorsak and Kravanja [82] and Smith et al. [81]. Stochastic methods for the retrofit design of heat exchanger networks have been presented by Bochenek and Jezowski [14], Ravagnani et al. [76] and Athier et al. [8].

The basic assumptions of HENS, such as the assumption of constant specific heat capacity, have been challenged. More detailed models for heat exchangers (pressure drop, heat exchanger type) have also been introduced. In Polley et al. [73] and Polley and Shahi [72] a relationship between the pressure drop and the individual heat transfer coefficients was proposed. Frausto-Hernández et al. [33] presented an MINLP model for HENS that considered pressure drop effects. Mizutani et al. [63] presented a Mathematical Programming model for the design of shell and tube heat exchangers and Mizutani et al. [64] used this work to develop a HENS model. Ravagnani and Caballero [75] presented a bilevel decomposition algorithm for HENS based on an MINLP model, where one level optimizes the HEN and the other level considers the detailed design of heat exchangers.

Another extension to basic HENS is heat integration between processes. Heat integration between processes can be considered as normal heat transfer between hot and cold process streams, but so that streams have specific processes to which they belong. These processes or process parts typically have their own specific processing tasks and sometimes are even owned by different companies. Heat transfer between different processes or process parts can be accomplished directly between process streams or with intermediate streams. Intermediate streams are used in order to reduce the number of transfer units between processes, because of the physical distance between the processes or for reasons of operational flexibility. Ahmad and Hui [4] were the first to study the problem of heat integration between processes or areas of integrity as they called it. They developed a systematic but sequential thermodynamic procedure for designing minimum energy networks which feature few interconnections between the areas or processes. In their procedure the designer can define if heat transfer between different processes occurs directly between streams or indirectly using isothermal intermediate streams. Hui and W. Ahmad [44] continued this work by integrating energy-capital trade-off calculations to these heat transfer situations. Another continuation of the original work was done by Hui and W. Ahmad [45], where the heat transfer between different processes was allowed only indirectly, with different levels of steam being used as the intermediate heat transfer streams. In that work they also developed a costing approach for the usage of steam that based on the graphical targeting tools of Pinch Technology. Dhole and Linnhoff [23] developed the concept into total site targets for fuel co-generation, emissions, and cooling. In their work heat integration between processes is allowed only indirectly with different steam levels as the intermediate streams. Only surplus heat, found by using Grand Composite Curves, could be transfered to other processes. They also developed other graphical tools based on pinch analysis for the problem. Amidpour and Polley [5] developed a zonal problem table algorithm which is a refinement of the Problem Table algorithm of Pinch Technology for the heat integration of different process parts. A total cost targeting procedure was also presented in their work, but no indirect heating using intermediate streams was allowed. Rodera and Bagajewicz [77] developed an energy-targeting procedure for heat integration between two processes. In their work heat could be transferred directly between streams in different processes or with intermediate streams that did not need to be isothermal. They also developed an optimization model for determining the optimal location of the fluid circuits in indirect heat exchanging. Bagajewicz and Rodera [9] extended this work to systems with more than two processes. No energy-capital trade-off calculations were performed in either of these studies. Kralj et al. [48] presented a three-step optimization method for heat integration between processes. In their approach optimization in the last step was performed by simultaneous heat integration inside and between the different processes. The first two steps, which are optional, try to simplify and direct the search towards desired good results. In their work no indirect heat transfer is possible, so their optimizing method can be considered as a basic heat exchanger network synthesis method. In the final step they used the Synheat model for HENS.

One reason for developing special methods and models for heat integration between processes is to keep the resulting heat exchanger networks as flexible as possible while increasing the energy efficiency. This can also be accomplished by developing flexible heat exchanger networks and for this reason a lot of work has been done on this field. One of the first studies of this problem was by Floudas and Grossmann [30], who developed a multi-period version of the mixed integer linear programming (MILP) transshipment model that accounts for the changes in pinch points and utility requirement during each time period. In their systematic procedure network configurations that require the minimum utility cost for each period of operation and involve the smallest number of units can be found. Floudas and Grossmann [31] developed an optimization method where the problem is decomposed into two stages: (i) prediction of matches; (ii) derivation of the network configuration. At each stage, synthesis techniques are combined with a flexibility analysis to test the feasibility of the operation of the design over a specified range of uncertain parameters. Tantimuratha et al. [83] presented a conceptual tool to address the flexibility and operability objectives for heat exchanger networks. In their approach a screening model to accommodate the flexibility considerations ahead of design was presented. Aaltola [1] presented a systematic framework that is based on the multiperiod MINLP model of Yee and Grossmann [89] for generating flexible heat exchanger networks over a specified range of variations in terms of the flow rates and temperatures of the streams. In this framework feasibility was tested after the network generation using a feasibility model. Konukman et al. [47] presented a non-iterative, superstructure-based, simultaneous MILP formulation for HENS synthesis where predefined flexibility targets are included in HENS. In their approach only source-stream temperatures are considered to be uncertain input parameters in order to keep the convexity assumption needed in their approach. Verheyen and Zhang [86] made modifications to the work of Aaltola [1], including the use of maximum area per period in the area cost calculation of the MINLP objective function and the removal of slack variables and weighed parameters from the existing NLP improvement model.

Integrated process-network synthesis (PNS and HENS) approaches have also been presented, although integrating two extremely complicated tasks cannot be accomplished easily. The works by Duran and Grossmann [25], Lang et al. [49], Yee et al. [91], Grossmann et al. [37], and Nagy et al. [66] belong to this group.

In this thesis the models and methods developed are aimed at greenfield design not retrofit design. Even though the latter is not studied, the models and methods should also be able to solve retrofit situations. In this thesis all the models and methods assume a constant specific heat capacity and heat transfer coefficients for the streams. Basic countercurrent heat exchangers are assumed, without considerations of pressure drop or type. In this thesis a model for heat integration between processes is presented in Publication I. The special features of this model are the simultaneous synthesis of heat exchanger networks which allow direct heat transfer between streams in the same processes and the fact that both direct and indirect heat transfer between process streams are included. In some of the above-mentioned works this is accomplished sequentially with pinch analysis-based tools, but this can easily lead to the best solutions being cut off, especially because the energy targeting phase too is decomposed into sequential steps. Multiperiod considerations have not been taken into account, although in general there should not be any reason why the models and methods in this thesis could not be applied in multiperiod situations as well.

3. Methods

Chapter 3 presents the different optimization methods and models developed in this thesis. Chapter 1.6 and Figure 1.4 have already presented how these methods are connected to each other and why these methods needed to be developed.

3.1 A mathematical optimization model for heat integration between and inside process sections /Indirect/

Chapter 3.1 presents a MINLP model (called *Indirect*) for HENS that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes. This model is useful for situations where the possibilities for heat integration between process sections need to be analyzed and optimized. This situation occurs because process plants are typically divided into different process parts that have specific processing tasks and possibly different ownership. Heat integration between these processes can increase the energy and economic efficiency of both the plant overall and the individual processes. The indirect heat transfer is accomplished by using intermediate streams. Intermediate streams are used in order to reduce the number of transfer units between processes, because of physical distance between the processes and for reasons of operational flexibility.

The objective of heat integration between different processes is to develop heat exchanger networks that minimize the annual energy and investment costs while also considering issues related to the existence of different processes. The main objective of the model in Chapter 3.1 is not to provide a new computationally efficient HENS method, but to provide a new HENS model that is specially directed to situations where a process plant is divided into specific processes. In this case the streams are

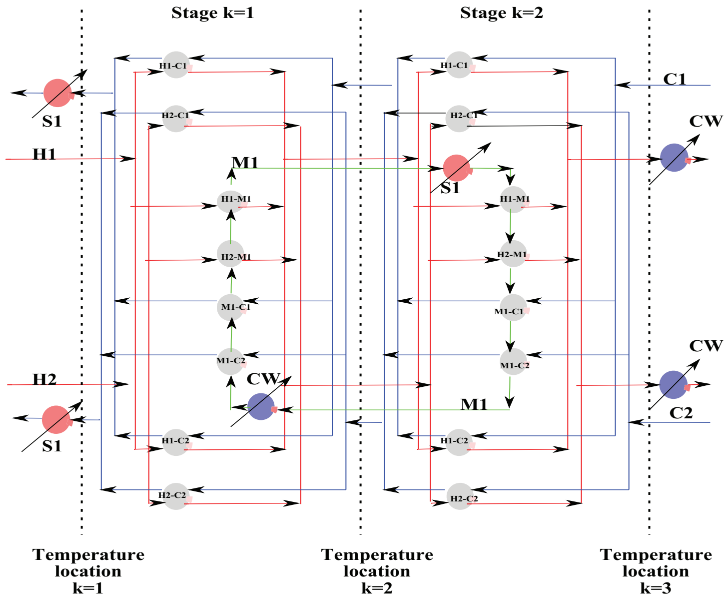

Figure 3.1. Superstructure for two hot and two cold process streams and one intermediate stream in two stages.

grouped according to the topological fact that different streams exist in different processes. The weighting method using fixed weights (annual costs) is the multiobjective approach used to solve the problem, because in this way the results can easily be compared to the results obtained with other methods.

3.1.1 Model

The model uses the stagewise superstructure proposed by Yee and Grossmann [89] as the basis for modeling. In this work the superstructure is modified in such a way that an additional index is given that indicates which process a stream belongs to. The indirect intermediate streams are introduced as streams not included in the process streams. The variables that are optimized are the temperatures in each stage of all streams, including the intermediate streams. The objective function, i.e., the total annual cost of the network, is dependent on these temperatures. The heat capacity flow rate, FCp, of the intermediate streams is assumed to be so big that the temperature of the stream does not change by heating or cooling (e.g., boiling of water). In this way the temperature of the intermediate stream is not dependent on the amount of heat the intermediate streams exchange. In a specific process only heating or cooling, not both, is allowed for a specific intermediate stream. In order to keep the energy balance of an intermediate stream, the overall heating and cooling of an intermediate stream must be equal to zero, i.e., if the intermediate stream is heated in one process, it has to be cooled equally in other processes or cooled with utilities. Hot and cold utilities can be used both for process and intermediate streams. Figure 3.1 shows the superstructure with two hot and two cold process streams and one intermediate stream.

Detailed equations defining the model can be found in Publication I of this thesis.

3.2 HENS with a bilevel optimization method /SingBilevelII/

Chapter 3.2 presents a simultaneous HENS method (called *SingBilevelII*) that uses bilevel optimization, stream data grouping, and the aggregation of streams. The objective of the method is to generate good solutions for HENS in a computationally efficient way so that all the objectives of HENS are optimized simultaneously. The models of the method are based on the Synheat superstructure presented by Yee and Grossmann [89]. The idea of the method is to decompose the set of binary variables, i.e., the variables that define the existence of heat exchanger matches, into two separate problems. In this way the number of different options to connect the streams decreases compared to the situation where no decomposition is present. The solution time should also decrease, which is also shown in two of the examples presented in Chapter 4.2.

The weighting method with fixed weights is the multiobjective approach used, so the overall objective is to minimize the total annual cost of the heat exchanger network. This is done in order to compare the results obtained to the ones found in the literature.

The method that is presented combines four mathematical programming models into an overall method. In the first step, first the number of groups is decided with Equation 3.1 and with this information, using *Submodel-1*, the process streams are organized into separate groups. In the second model, *Submodel-2*, hot and cold aggregate streams for each group are formed from each groups hot and cold process streams. This model is a non-linear model (NLP). The third model, *Submodel-3*, which is a mixed integer non-linear model (MINLP), minimizes the total annual cost of the heat exchanger network, but in such a way that direct heat exchanging between streams in different groups is not allowed. This means that the hot streams of a specific group can exchange heat only with the cold streams in the same group and with the cold aggregate streams of other groups. Hence direct heat exchanging between streams in different groups is not allowed. Process streams and aggregate streams can also exchange heat with utility streams. In the fourth model, *Submodel-4*, which is a mixed integer non-linear model (MINLP), all hot streams are allowed to exchange heat with all cold streams, but in such a way that the binary variables indicating the existence of heat exchanging matches between streams in the same group are fixed according to the results obtained from *Submodel-3*. As a result of non-convexities in the model and due to the decomposition approach, the initial solution might not be optimal, so in order to achieve a good solution the procedure continues by adding integer cuts to *Submodel-3* and iterating *Submodel-3* and *Submodel-4* until a good solution is obtained. In this work the iterations terminate when a satisfactory result has been obtained. In the method that is presented a solution is satisfactory if the values of both *Submodel-3* and *Submodel-4* start to increase compared to any previous iterations. In this way the probability of being trapped in a local optimum decreases. So as a consequence at least two major iterations are always solved.

Figure 3.2 shows the different steps of the overall method.

Detailed mathematical models of the submodels, together with the definitions of the indices, sets, parameters and variables are presented in Publication III of this thesis.

$$\begin{aligned} structures = \Big(& \sum_G (\text{number of hot streams in group} \cdot \text{number of cold streams in group}) \\ & + (\text{number of hot streams in group} \cdot (\text{number of groups - 1}) \\ & + (\text{number of cold streams in group} \cdot (\text{number of groups - 1})\Big)^2 \\ & + \Big(\sum_G (\text{number of hot streams in group} \cdot \text{number of cold streams in other groups})\Big)^2 \end{aligned} \tag{3.1}$$

3.2.1 Submodel-1 of SingBilevelII

In the first step of the method, the objective is to distribute the process streams into groups g. This is done by first defining the number of groups

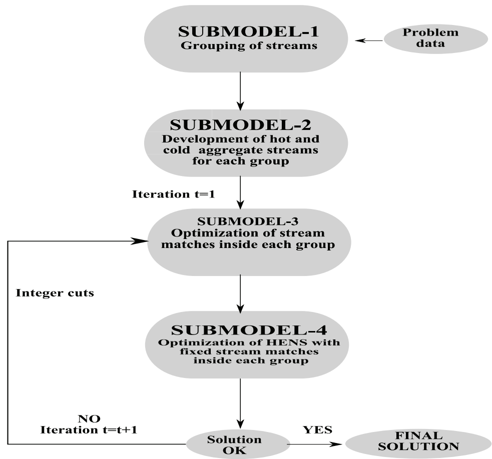

Figure 3.2. Flowsheet of the overall *SingBilevelII* method combining the four submodels

and calculating how many hot and cold process streams there are in each group. With this information the hot and cold streams are distributed into different groups.

he minimum number of groups is two and the maximum number of groups is the minimum number of either hot process streams or cold process streams. So if there are four hot streams and five cold streams, there can be two, three, or four groups. Both hot and cold streams are distributed evenly to the groups. This means that all groups have at least one hot and one cold process stream. As an example, for the case with four hot streams and five cold streams and if the number of groups is two, in the first group there will be two hot process streams and three cold process streams and in the second group there will be two hot streams and two cold streams. If the number of groups is three in the same example, in the first group there will be two hot streams and two cold streams, in the second group there will be one hot stream and two cold streams, and in the third group there will one hot stream and one cold stream.

The number of groups can be a user-given parameter or estimated according to the maximum number of possible heat exchanger matches. The latter approach is used in this work. The objective here is to minimize the number of possible heat-exchanging matches between hot and cold process streams or, to be even more precise, the possible structures in the network. For example, if a problem has 10 hot streams and 10 cold streams and no grouping is used, i.e., normal direct heat exchanging is allowed (not using the proposed method), the number of groups is 1, no aggregate streams are present and the maximum number of possible heat exchanger matches is $10 \times 10 = 100$ in the first optimization level and 0 in the second optimization level (only one optimization level). So altogether there are $2^{100} + 0 = 1.268 \cdot 10^{30}$ different optional structures. On the other hand, if there are two groups which both have five hot and five cold streams, one hot and one cold aggregate stream are needed for both groups and the total amount of possible heat exchanger matches is $(5 \times 5 + 5 \times 5 + 5 \times 1 + 5 \times 1) = 70$ possible matches on the first optimization level and $(2 \times 5 \times 5) = 50$ on the second optimization level, resulting in $2^{70} + 2^{50} = 1.181 \cdot 10^{21}$ different optional structures. If there are five groups that each have two hot and two cold streams, one hot and one cold aggregate stream are needed for each group and the total amount of possible heat exchanger matches is $(5 \times 2 \times 2 + 5 \times 2 \times (5-1) + 5 \times 2 \times (5-1) = 100$ on the first optimization level and $(5 \times 2 \times 8 = 80)$ on the second optimization level, resulting in $2^{100} + 2^{80} = 1.27 \cdot 10^{30}$ different optional structures. The smallest number is chosen as the number of groups. This estimation does not consider the fact that typically not all hot streams can exchange heat with all cold streams (if a cold stream is hotter than a hot stream). Equation 3.1 shows how the number of possible structures is calculated for a chosen number of groups. In this way the traditional non-grouping or having only one group can be seen as a special grouping approach.

After the number of groups and how many streams there are in each group have been decided, the decision as to which streams go into which groups needs to be solved. This is done in such a way that each stream is forced to exchange all of its heat with a reference stream and the area cost of the heat exchanger that is needed to accomplish this task, is calculated, providing a reference value, *ref*, for each stream. The reference stream is a stream that has an appropriate temperature level for heat exchanging. For cold process streams the reference stream has a temperature t higher than any of the target temperatures of the cold process streams, and for the hot process streams the reference stream has a temperature, t, cold enough that all the target (end) temperatures of the hot process streams have higher temperatures. In the method that is presented, the hot utility, HU, is used as a hot reference stream for the cold process streams and the cold utility, CU, as a cold reference stream for the hot process streams.

The reference values, ref_i and ref_j (area costs), are calculated with

Submodel-1. The approximation of the logarithmic mean temperature difference (lmtd) is by Paterson [70] and it is used in all the models.

After *Submodel-1* has been solved, the hot and cold process streams are ordered according to their reference values. The hot streams are distributed into the groups, in such a way that the hot process streams with the largest reference values go into group number 1 and the hot process streams with the smallest reference values go into the last group. So process streams have reference values that are as similar as possible in each group. As an example it is assumed that there are five hot process streams altogether and, assuming that there are two groups (according to Equation 1), the three hot process streams with the largest reference values will go into group number 1 and the two hot process streams with the smallest reference values will go to group number 2. If Equation 3.1 had defined that there are three groups, then group number 1 will have two hot process streams (the ones with the biggest reference values found with *Submodel-1*), two hot process streams will go into group number 2 (the ones with the third and fourth biggest reference values) and one hot process stream (the one with the smallest reference value) will go into group number 3. The same kind of procedure is carried out for the cold process streams.

3.2.2 Submodel-2 of SingBilevelII

After the streams have been distributed into groups, hot and cold aggregate streams are developed from the hot and cold process streams existing in each group. The objective is to develop an aggregate stream that has similar properties to the streams it represents. In this way there will be only one stream, i.e., the aggregate stream, that acts like the process streams it represents. An aggregate stream has investment costs (heat transfer area costs and fixed unit costs) less than or equal to the sum of the investment costs of the process streams it represents. The investment costs of both the aggregate stream and the process streams that the aggregate stream represents are calculated, with the assumption being made that the streams exchange heat with a reference stream. All other properties (the amount of heat in this case) are the same for the aggregate stream and the process streams that the aggregate stream represents. In this work the hot and cold reference streams are chosen to be the hot and cold utility streams. So the basic idea is to find optimum values for the start temperature, tin, end temperature, $tout$, heat capacity flowrate, fcp, and heat transfer coefficient, h, of an aggregate stream so that its investment cost is equal to the sum of the investment costs of process streams it represents. This is with the assumption that all streams exchange heat with a reference stream.

Initial values and bounds

The aggregate streams are imaginary streams whose purpose it is to resemble, regarding the investment costs and amount of heat, the process streams they represent as closely as possible. Hence start temperatures, tin, end temperatures, $tout$, heat capacity flow rates, fcp, and heat transfer coefficients, h, are positive variables that need initial values, upper bounds, and lower bounds.

In the method that is presented the start temperature of a hot aggregate stream is the highest start temperature of the hot process streams it represents and the start temperature of a cold aggregate stream is the lowest start temperature of the cold process streams the aggregate stream represents. The end temperature of an aggregate stream is between the maximum and minimum end temperatures of the process streams the aggregate stream represents. The minimum heat capacity flow rate of an aggregate stream is between the smallest flow rate of the process streams the aggregate stream represents and the sum of the maximum flow rates of the process streams the aggregate stream represents. The heat transfer coefficient of an aggregate stream is chosen to be as free as possible, so that the objective function value of *Submodel-2* is as close to zero as possible. Hence, the lower bound chosen in this work is just above zero (0.01) and the upper bound is $10\times$ the biggest heat transfer coefficient value. The initial values of the aggregate stream variables are always on the lower bound.

After *Submodel-2* is solved, these optimized values are fixed in the subsequent steps. So in the next steps, tin, $tout$, fcp, and h of the aggregate streams become parameters TIN, $TOUT$, FCpn and H.

3.2.3 Submodel-3 of SingBilevelII

In the third stage of the method, the heat exchanger network is synthesized so that heat can be exchanged between process streams in the same group, between process streams and aggregate streams which are not in the same group, process streams and utility streams and aggregate streams and utility streams. No cost is assigned for the aggregate-to-utility stream matches. The only merit of these matches is that they enforce energy balances for the aggregate streams too. The objective of *Submodel-3* is to find the correct process-to-process heat exchanger matches in each group, because these values are fixed in the final stage of the method. The objective function minimizes the total annual cost of the network.

3.2.4 Submodel-4 of SingBilevelI

The final step of the methodology is the synthesis of the network, but in such a way that the existence or non-existence of heat-exchanging matches of process streams in the same group is fixed according to the results of *Submodel-3*. This final step is provided by *Submodel-4*. *Submodel-4* is equivalent to the basic Synheat model by Yee and Grossmann [89].

3.3 Interactive multiobjective approaches to HENS

In Chapter 3.3 two different approaches to HENS using NIMBUS, the interactive multiobjective optimization method, are presented. In the first approach the basic Synheat model was used to test the applicability of NIMBUS for solving HENS problems. In this case no stream grouping is used. This HENS approach introduces a new tool called the A–GAMS–NIMBUS-tool, which integrates IND-NIMBUS with the GAMS modeling system. This enables GAMS to be used for solving multiobjective optimization problems without weighting factors being used. This A–GAMS–NIMBUS tool can easily be applied to fields outside HENS.

The second interactive multiobjective optimization approach for HENS uses the A–GAMS–NIMBUS-tool together with the bilevel approach presented in Chapter 3.2 providing a designer of heat exchanger networks a robust and computationally efficient HENS method in which the designer of a network can guide the design procedure to the areas of most interest with information that is understandable to the designer. In this thesis the method is called MOBilevelI.

In both approaches, four objective functions are minimized:

- the number of heat exchanger units
- the total heat exchanger surface area
- hot utility consumption
- cold utility consumption

As can be seen, the different utility consumptions are treated as different objectives, although in most cases they correlate strongly. But this is not always the case, and with this approach the DM can decide which utility consumption is more important. In both approaches, all the steps or submodels are such that cost functions for the heat exchanger network are not needed.

3.3.1 An interactive multi-objective optimization method for HEN synthesis /A–GAMS–NIMBUS-tool/

This section presents an integration of GAMS and IND-NIMBUS. A simplified implementation of the NIMBUS method is applied and the tool is called the A–GAMS–NIMBUS-tool.

NIMBUS method implementation with GAMS

IND-NIMBUS is a multi-platform desktop application for implementing the NIMBUS method. The NIMBUS method is an interactive multiobjective optimization method, that is, new Pareto optimal solutions are produced during the optimization process following the preference information provided by the DM (Miettinen [59], Miettinen and Mäkelä [62]). Previously, the NIMBUS method has been applied to the optimal shape design of ultrasonic transducers (Heikkola et al. [42]), designing a paper machine headbox (Hämäläinen et al. [41]), optimal control in the continuous casting of steel (Miettinen [61]), the separation of glucose and fructose (Hakanen et al. [39]), intensity modulated radiotherapy treatment planning (Ruotsalainen et al. [78]), brachytherapy (Ruotsalainen et al. [79]), and wastewater treatment design (Hakanen et al. [40]), among others. When using the NIMBUS method, the DM is asked to provide his or her preference information by classification of the objective functions. This classification information is used to formulate the multiobjective problem as a scalarized single-objective problem, and solving this problem provides the DM with a new Pareto optimal solution(s) and the DM can see how well the desired changes in the objective function values could be achieved. IND-NIMBUS does not contain any tools to formulate the optimization problem. Therefore it must be connected to external simulation or modeling software in order to be used for solving any multiobjective optimization problems. In the A–GAMS–NIMBUS-tool, the DM can use the graphical user interface developed for the IND-NIMBUS software to solve multiobjective optimization problems expressed with the GAMS modeling language, utilizing single-objective solvers provided in the GAMS software.

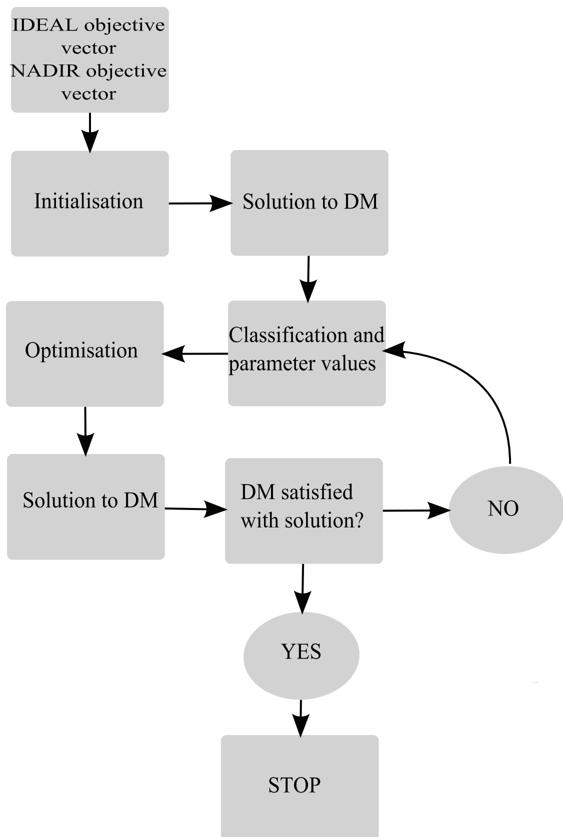

Figure 3.3. Outline of integrated NIMBUS–GAMS-tool

The procedure of the A–GAMS–NIMBUS-tool can be seen in Figure 3.3. The steps of the method are presented in the following sections. A detailed model and indices, sets, parameters, and variables of the method are presented in Publication IV of this thesis. A screenshot of the A–GAMS–NIMBUS-tool can be seen in Figure 3.4.

Step 1: Initialization

As a first step of NIMBUS, estimated upper and lower bounds of objective values in the set of Pareto optimal solutions are calculated. They are called *nadir* and *ideal* objective vectors, respectively. The Synheat model is solved for all four objectives separately so that one objective at a time is minimized and the values of the other objectives are calculated, but not optimized. The ideal objective value f_o^* for a specific objective is the value that is obtained when that specific objective is minimized. The components of the *nadir* objective vector f_o^{nad} are then estimated using a payoff table (see, e.g., Miettinen [59]). We define $f_o^{**} = f_o^* - \varepsilon$ for each i, where $\varepsilon > 0$ is a small scalar.

Next, the first (weakly) Pareto optimal solution must be calculated for the first classification step. This can be done by solving the following scalarized problem (3.2).

$$
\begin{aligned}
&\min \alpha \\
&\text{subject to } \alpha \geq \frac{f_o(\mathbf{x}) - f_o^*}{f_o^{nad} - f_o^{**}} \qquad \text{for all } o \text{ functions} \\
&\mathbf{x} \in S.
\end{aligned}
\tag{3.2}
$$

Solving the initialization phase provides a first (weakly) Pareto optimal solution.

Step 2: Classification

In the first classification step, the initial solution is presented to the DM. Then the DM has to decide into which classes the different objective functions are assigned.

NIMBUS has five classes into which objectives can be classified. For a minimization problem, the different classes are:

functions f_o

- $I^{<}$ whose value should be minimized as much as possible,
- $I^{\leq}$ whose value should be minimized till a desired aspiration level $\hat{f}_o$,
- $I^{\geq}$ whose value can increase till a specified upper bound E_o,
- $I^{=}$ whose value is acceptable and
- $I^{\diamond}$ whose value can be changed freely.

It is naturally possible to use only some of the five classes available. In any case, because the solution to be classified is Pareto optimal, when making a classification the DM must allow some of the objectives to get worse in order to allow some others to improve in value. Thus, classes $I^{<}$ or $I^{\leq}$ and classes $I^{\geq}$ or $I^{\diamond}$ cannot be empty.

Additionally, if an objective function is assigned to the class $I^{\leq}$, the DM has to give an aspiration level $\widehat{f}_o$ (which is lower than the current objective value) and if an objective function is in the class $I^{\geq}$, the DM has to give the upper bound value E_o (which is higher than the current objective value).

The so-called synchronous NIMBUS algorithm uses altogether four different scalarized problems to generate several new Pareto optimal solutions for the given classification information. In the A–GAMS–NIMBUS-tool, only one scalarization problem, Model 3.3, is used.

$$\min \alpha \tag{3.3}$$

subject to

$$\alpha \geq \frac{f_o(\mathbf{x}) - f_o^*}{f_o^{nad} - f_o^{**}}, \qquad \text{for all } o \in \{I^{<}\}$$

$$\alpha \geq \frac{f_o(\mathbf{x}) - \widehat{f}_o}{f_o^{nad} - f_o^{**}}, \qquad \text{for all } o \in \{I^{\leq}\}$$

$$f_o(\mathbf{x}) \leq f_o^{jk*}, \qquad \text{for all } o \in \{I^{<}, I^{\leq}, I^{=}\}$$

$$f_o(\mathbf{x}) \leq E_o, \qquad \text{for all } o \in \{I^{\geq}\}$$

$$f_1(\mathbf{x}) = \text{Number of units}$$

$$f_2(\mathbf{x}) = \text{Total heat exchanger area}$$

$$f_3(\mathbf{x}) = \text{Total hot utility}$$

$$f_4(\mathbf{x}) = \text{Total cold utility}$$

$$\mathbf{x} \in S.$$

Here, the index *j** refers to current objective function values. For example, for the first classification step, f_i^{j*} represents the value of f_i obtained by solving the problem (3.2) during the initialization step. S is defined by the constraints defined in Publication IV of this thesis and in Yee and Grossmann [89].

Classification can be performed with the user-interface of IND-NIMBUS. A screenshot of the A–GAMS–NIMBUS-tool can be seen in Figure 3.4. Here, on the left-hand side of the window, the DM can classify objective functions by clicking colored bars, each representing an objective function. Below each bar, the DM can see the current values of the objective functions, and function value ranges are shown on the right- and left-hand sides of the bars. On the right-hand side of the window, the DM is shown all the previously calculated Pareto optimal solutions and promising solutions can be located at the bottom part.

For making a new classification, the DM can classify either by starting with the currently selected solution, or by selecting any previously found Pareto optimal solution as the current solution. The classification is done by simply clicking different parts of the objective function bar, depending on how the DM wishes to change the objective values of the currently selected solution. If the value is desired to be reduced as much as possible ($f_o \in I^{<}$), the arrow pointing to the left is clicked, or if the value is desired to change freely, one can leave it unclassified or click the arrow pointing to the right ($f_o \in I^{>}$). If the DM desires to give some upper or lower boundary ($f_o \in I^{\leq}$ or $I^{\geq}$), the actual bar can be clicked and the corresponding value can then be edited in the edit box next to the function bar. If the current objective function value is considered to be acceptable, the arrow pointing downwards can be clicked ($f_o \in I^{\diamond}$).

After the DM is satisfied with the classification, she/he can get a new Pareto optimal solution by pressing the green play button. To be more specific, the A–GAMS–NIMBUS-tool then formulates a GAMS model as described earlier, and instructs the GAMS environment to solve the model and presents the DM with the results that have been obtained earlier, i.e., with the new Pareto optimal solution. The DM can then either use this new solution as the basis for a new classification, or continue by selecting some other, previously found solution. By continuing in this way, the DM can generate various Pareto optimal solutions according to her/his preferences, learn about interdependencies among the objectives, and what kind of solutions are attainable and eventually identify the most preferred solution by using intuitive preference information.

After the scalarized problem (3.3) has been solved, the values of the different objective functions are provided to the DM. If the DM is satisfied with the result, the optimization procedure stops. If not, the DM provides new classes (and aspiration levels and upper bounds if needed) and problem (3.3) is solved again.

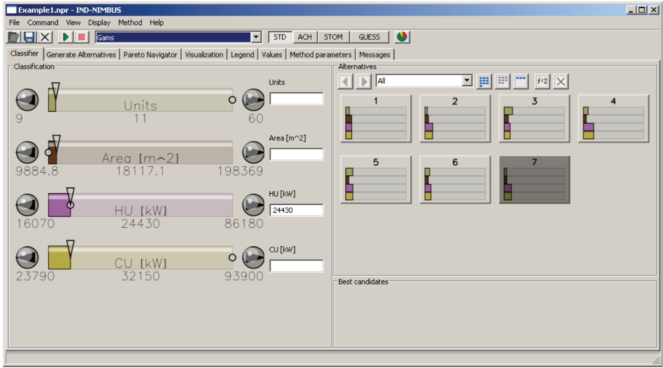

Figure 3.4. A–GAMS–NIMBUS-tool classification window

3.3.2 Bilevel interactive multiobjective HENS method /MOBilevelI/

As presented in Publication III, the objective of the original single-objective bilevel optimization method SingBilevelII is to decompose the set of binary variables *i.e.* the variables that define the existence of heat exchanger matches, into two separate problems. This same approach is also used in the method presented in this chapter, but here the simplified version of the synchronous NIMBUS method of [62] is used to optimize the heat exchanger network as a genuine multiobjective optimization problem.

Overall method of MOBilevelI

The overall calculation method is depicted in Figure 3.5.

The steps of the overall procedure involving the NIMBUS method are the following.

- *Grouping of streams.* As a first step the problem data is used to calculate the number of groups and to define which process stream goes into which group (*Equation 3.1 in Chapter 3.2.1 and Submodel-1* of Publication V).

- *Aggregate streams.* Using *Submodel-2* of Publication V, hot and cold aggregate streams for each group are formed from the hot and cold process streams in that group. These aggregate streams are imaginary streams that try to resemble the sum of the process streams that they represent regarding start temperatures, end temperatures, heat capacity flow rates and heat transfer coefficients.

- *Ideal and Nadir vectors.* Next, *ideal* and *nadir* objective vectors are found using *Submodel-4* of Publication V. The *ideal* and *nadir* objective vectors are the estimated upper and lower bounds of objective function values in the set of Pareto optimal solutions. *Submodel-4* of Publication V is used to find the best value of each objective function by ignoring the others. By optimizing each objective function at a time we get an ideal objective value f_o^* for each objective f_o. The components of the *nadir* objective vector f^{nad} are then estimated using a payoff table (see, e.g. [59]). We define $f_o^{**} = f_o^* - \varepsilon$ for each o, where $\varepsilon > 0$ is a small scalar.

- *Initial Pareto optimal solution.* In the next step, a Pareto optimal solution is generated as a starting point for the interactive NIMBUS method. This is done without input from the DM, by using Equation 3.5 with a reference point $\hat{f}_o = \frac{f_o^{nad} + f_o^{**}}{2}$. This so-called neutral compromise solution is obtained by solving the bilevel part of the method. First, *Submodel-3* of Publication V optimizes the heat exchanger network, but in such a way that the hot (cold) streams of a specific group can exchange heat with the cold (hot) streams in the same group and with the cold (hot) aggregate streams of other groups. Hence, the direct exchanging of heat between streams in different groups is not allowed. Process streams and aggregate streams can also exchange heat with utility streams. Then in *Submodel-4* of Publication V all hot streams are allowed to exchange heat with all cold streams, but in such a way that the binary variables indicating the existence of heat-exchanging matches between streams in the same group are fixed according to the results obtained from *Submodel-3* in Publication V. The procedure continues by adding binary cuts in *Submodel-3*, and solving it and the following *Submodel-4* repeatedly over again until a satisfactory result is achieved. A solution is satisfactory when the optimal values (variable α) of *Submodel-3* and *Submodel-4* have started to increase compared to previous iterations or the models are infeasible. The result of all the solutions of *Submodel-4* that best satisfies the DM is chosen as the initial solution of the overall method. In theory, the results of *Submodel-4* in other minor iterations can also be locally Pareto optimal, so basically any minor iteration solution could be used as an initial solution.

- *Classification.* In this step the DM is asked to classify the objectives of the currently selected Pareto optimal solution in order to indicate how to make the solution better. As mentioned, there are five classes into which objectives can be classified.

- *Bilevel optimization.* *Submodel-3* is solved with this classification. Before *Submodel-3* is solved, the minor iteration loop count tk is initialized to the value 1 and the major iteration loop count jk is initialized to the value 2, because the initial solution is considered to be the first major iteration. After *Submodel-3* has been solved, the binary variables indicating the existence of heat exchanger matches between streams in each group are fixed and *Submodel-4* is solved. Next, *Submodel-3* is solved again with integer cuts added, so that previous results are excluded from the possible solutions. Then *Submodel-4* is solved with the new fixed binary variables. This procedure continues until a satisfactory solution has been found. A solution is satisfactory when the optimal values (variable α) of *Submodel-3* and *Submodel-4* have started to increase compared to previous iterations or the models are infeasible.

  The final solutions (*Submodel-4* solutions) are presented to the DM and the DM chooses one of these as the final solution of this major iteration. After this, the DM makes a new classification of the objectives and the calculation procedure continues to the major iteration $jk = 3$ with the minor iteration loop $tk = 1$. These major iterations are continued until the DM is satisfied with the result.

In MOBilevelI, all steps or submodels are such that cost functions for the heat exchanger network are not needed. Compared to the work in Publication III, *Submodel-3* and *Submodel-4* are changed from single-objective optimization to multiobjective optimization. This is done on the basis of the simplified version of the interactive NIMBUS method (see Publication IV), although in this case, additionally, an augmentation term is added to the scalarization functions in order to provide (locally) Pareto optimal solutions and also two scalarization functions are used compared to just one, as was the case in Publication III (Equations 3.4 and 3.5). In NIMBUS, scalarization functions are formed on the basis of the original multiobjective optimization formulation and the classification information provided by the DM. Optimal solutions of these single-objective scalarization functions are Pareto optimal for the original problem and they reflect the desires of the DM as closely as possible.

$$\min \alpha + \rho \sum_{o \in O} \frac{f_o(\mathbf{x})}{f_o^{nad} - f_o^{**}} \tag{3.4}$$

subject to

$$\alpha \geq \frac{f_o(\mathbf{x}) - f_o^{*}}{f_o^{nad} - f_o^{**}}, \qquad \text{for all } o \in \{I^{<}\}$$

$$\alpha \geq \frac{f_o(\mathbf{x}) - \widehat{f}_o}{f_o^{nad} - f_o^{**}}, \qquad \text{for all } o \in \{I^{\leq}\}$$

$$f_o(\mathbf{x}) \leq E_o, \qquad \text{for all } o \in \{I^{\geq}\}$$

$$f_1(\mathbf{x}) = \text{Amount of units}$$

$$f_2(\mathbf{x}) = \text{Total heat exchanger area}$$

$$f_3(\mathbf{x}) = \text{Total hot utility}$$

$$f_4(\mathbf{x}) = \text{Total cold utility}$$

$$\mathbf{x} \in S$$

$$\alpha \in R.$$

$$\min \alpha + \rho \sum_{o \in O} \frac{f_o(\mathbf{x})}{f_o^{nad} - f_o^{**}} \tag{3.5}$$

subject to

$$\alpha \geq \frac{f_o(\mathbf{x}) - \bar{f}_o}{f_o^{nad} - f_o^{**}}, \qquad \text{for all } o \in O$$

$$f_o(\mathbf{x}) \leq E_o, \qquad \text{for all } o \in \{I^{\geq}\}$$

$$\bar{f}_o = f_o^{*} \text{ for all } o \in \{I^{<}\}$$

$$\bar{f}_o = \widehat{f}_o \text{ for all } o \in \{I^{\leq}\}$$

$$\bar{f}_o = E_o \text{ for all } o \in \{I^{\geq}\}$$

$$\bar{f}_o = f_o^{jk*} \text{ for all } o \in \{I^{=}\}$$

$$\bar{f}_o = f_o^{nad} \text{ for all } o \in \{I^{\diamond}\}$$

$$f_1(\mathbf{x}) = \text{Amount of units}$$

$$f_2(\mathbf{x}) = \text{Total heat exchanger area}$$

$$f_3(\mathbf{x}) = \text{Total hot utility}$$

$$f_4(\mathbf{x}) = \text{Total cold utility}$$

$$\mathbf{x} \in S$$

$$\alpha \in R.$$

Here, O is the index set of all objective functions and f_o^{jk*} refers to the current objective function value of f_o. Furthermore, x is a variable in the feasible region S. As introduced earlier, ranges of objective function values in the set of Pareto optimal solutions are represented by ideal (i.e., the best) objective function values f_o^* and by nadir (i.e., the worst) objective function values f_o^{nad} of each objective f_o. To avoid dividing by numbers that are too small, we use the utopian objective function values f_o^{**} instead of f_o^* in the denominators. The desired objective function values in the class $I^{\leq}$ are denoted by $\widehat{f}_o$ and the upper bounds for functions in the class $I^{\geq}$ by E_o. In Equations (3.4) and (3.5), the term multiplied by a small positive number ρ is used to avoid generating weakly Pareto optimal solutions (see, e.g., Miettinen [59]). The original scalarization functions are so called min-max functions, which are non-differentiable. Using the real-valued variable α is a way of formulating the problem as a differentiable one (assuming all the functions involved are differentiable). The other constraints in the problems guarantee that the classification information is taken into account. By solving the problems above, we get a (properly) Pareto optimal solution to the original problem, see; Miettinen and Mäkelä [62].

In *Submodel-3* the different functions f_o of Equation (3.4) are given in Equations (3.6) to (3.9) and the ones in *Submodel-4* are given in Equations (3.10) to (3.13).

$$
\begin{aligned}
f_1(\mathbf{x}) = & \sum_{g\in G, i\in GI, j\in GJ, st\in ST} z_{i,j,st} \\
& + \sum_{g\in G, ri\notin GRI, j\in GJ, st\in ST} z_{ri,j,st} \\
& + \sum_{g\in G, i\in GI, rj\notin GRJ, st\in ST} z_{i,rj,st} \\
& + \sum_{g\in G, i\in GI} z_{i,cu} \\
& + \sum_{g\in G, j\in GJ} z_{hu,j} & (3.6)
\end{aligned}
$$

$$
\begin{aligned}
f_2(\mathbf{x}) = & \sum_{g\in G, i\in GI, j\in GJ, st\in ST} \frac{q_{i,j,st}\cdot(\frac{1}{H_i}+\frac{1}{H_j})}{lmtd_{i,j}} \\
& + \sum_{g\in G, ri\notin GRI, j\in GJ, st\in ST} \frac{q_{ri,j,st}\cdot(\frac{1}{H_{ri}}+\frac{1}{H_j})}{lmtd_{ri,j}} \\
& + \sum_{g\in G, i\in GI, rj\notin GRJ, st\in ST} \frac{q_{i,rj,st}\cdot(\frac{1}{H_i}+\frac{1}{H_{rj}})}{lmtd_{i,rj}} \\
& + \sum_{g\in G, i\in GI, cu\in CU} \frac{q_{i,cu}\cdot(\frac{1}{H_i}+\frac{1}{H_{cu}})}{lmtd_{i,cu}} \\
& + \sum_{g\in G, j\in GJ, hu\in HU} \frac{q_{hu,j}\cdot(\frac{1}{H_{hu}}+\frac{1}{H_j})}{lmtd_{hu,j}} & (3.7)
\end{aligned}
$$

$$f_3(\mathbf{x}) = \sum_{j\in GJ} q_{hu,j} \quad (3.8)$$

$$f_4(\mathbf{x}) = \sum_{i\in GI} q_{i,cu} \quad (3.9)$$

$$f_1(\mathbf{x}) = \sum_{i\in I, j\in J, st\in ST} z_{i,j,st} + \sum_{i\in I} z_{i,cu} + \sum_{j\in J} z_{hu,j} \quad (3.10)$$

$$
\begin{aligned}
f_2(\mathbf{x}) = & \sum_{i\in I, j\in J, st\in ST} \frac{q_{i,j,st}\cdot(\frac{1}{H_i}+\frac{1}{H_j})}{lmtd_{i,j}} \\
& + \sum_{i\in I, cu\in CU} \frac{q_{i,cu}\cdot(\frac{1}{H_i}+\frac{1}{H_{hc}})}{lmtd_{i,cu}} \\
& + \sum_{j\in J, hu\in HU} \frac{q_{hu,j}\cdot(\frac{1}{H_{hu}}+\frac{1}{H_j})}{lmtd_{hu,j}} & (3.11)
\end{aligned}
$$

$$f_3(\mathbf{x}) = \sum_{j\in J} q_{hu,j} \quad (3.12)$$

$$f_4(\mathbf{x}) = \sum_{i\in I} q_{i,cu} \quad (3.13)$$

A–GAMS–NIMBUS-tool

In the A–GAMS–NIMBUS-tool, the simultaneous bilevel HENS problem is formulated as a multiobjective optimization problem and solved using the NIMBUS method. The classification information is used to formulate

Equations (3.4) and (3.5), using the GAMS modeling language, where the objective functions are defined either in *Submodel-3* or *Submodel-4*, depending on which level of the bilevel optimization method is being solved. These submodels are formulated using the GAMS modeling language, and therefore, single-objective solvers included within the GAMS software can be used to solve the multiobjective bilevel Synheat problem.

The DM could provide the classification information manually, for example using input files, but to have a more user-friendly approach, we use the A–GAMS–NIMBUS-tool software as a graphical user interface for the NIMBUS method, developed earlier in (Laukkanen et al. [50]). The A–GAMS–NIMBUS-tool is based on the IND-NIMBUS optimization software platform for developing interactive multiobjective optimization methods (see; Miettinen [60]).

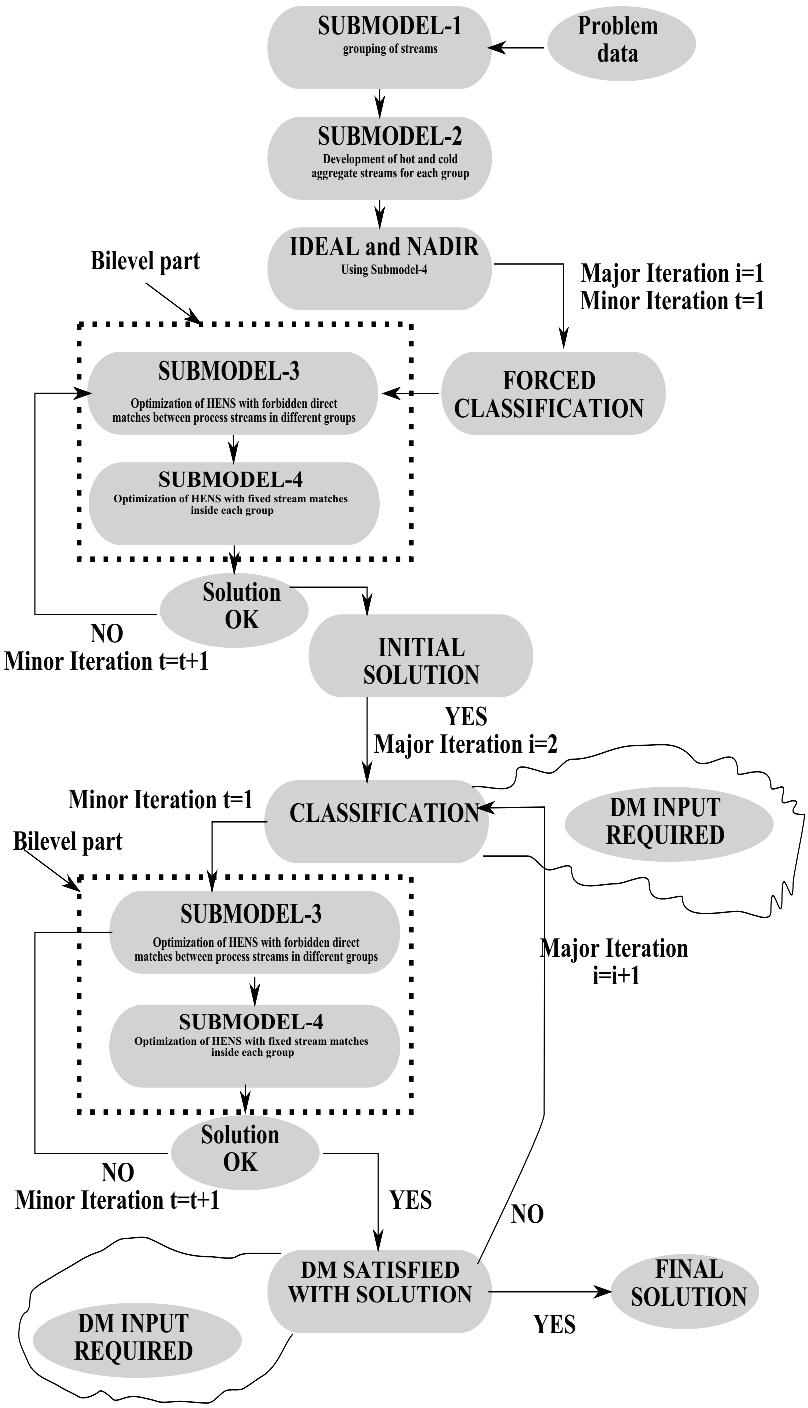

Figure 3.5. The overall MOBilevelI method

4. Results of examples solved with the methods

Chapter 4 presents solutions of examples that are solved with the models and methods presented in this thesis. The problems are solved with GAMS (Brook et al. [16]). The solvers used together with GAMS are shown in Table 4.1. All the mathematical programming problems were solved on a laptop with a mobile Intel Core 2 Duo T8300 NV 2.4-GHz processor. The flowsheets are drawn with HeVi (Publication VI), a software which can be downloaded from *http://eny.tkk.fi/hevi/* for free.

problem type:	solver(s):
MINLP	DICOPT[a]
NLP	CONOPT3[b]
MILP	CPLEX[c]

[a]Engineering Design Research Center (EDRC) at Carnegie Mellon University
[b]ARKI Consulting and Development A/S
[c]ILOG CPLEX Division

Table 4.1. Solvers for the optimization problems used in the examples.

4.1 Results of examples solved with the Indirect model

The model is used to optimize two examples. The first one is a small invented example and the second one is from Ahmad and Hui [4].

4.1.1 Indirect: Small example

The data of the small example are given in Table 4.2, which also shows which streams are in which processes. The flows are invented, but the cost parameters are obtained from Kralj et al. [48]. This example is an artificial example, which is only used to describe how the model works. The

Stream	TIN [°C]	TOUT [°C]	FCp [$\frac{kW}{°C}$]	H [$\frac{kW}{m^2 \cdot °C}$]	Process
H1	155	30	8.0	2	1
H2	80	40	15.0	2	2
H3	200	40	15.0	2	2
C1	20	160	20.0	2	1
C2	20	100	15.0	2	1
C3	20	200	15.0	2	2
HU	220	220	-	2	
CU	10	10	-	2	

Plant lifetime 7 years

Interest rate 8.0 (%/a)

Annuity factor 0.192072 (-)

HEX cost, streams in the same process(direct) [\$] $= 8600 + 670 \cdot A^{0.83}$ (A in m^2)

HEX cost, streams in diff. processes(direct) [\$] $= 2 * 8600 + 670 \cdot A^{0.83}$ (A in m^2)

HEX cost, streams in diff. processes(indirect) [\$] $= UNITC_A * 2 * 8600 + 670 \cdot A^{0.83}$ (A in m^2)

Annual Hot Utility cost [\$$/kW \cdot a$] $= 100$

Annual Cold Utility cost [\$$/kW \cdot a$] $= 10$

H for hot and cold intermediate streams [$\frac{kW}{m^2 \cdot °C}$] $= 5$

Table 4.2. Indirect: Process data for small example.

CASE	$UNITC_A$	T_{ha}	Int. str Q	Area	Unit	HU	Total cost
	[$-$]	[°C]	[MW]	[m^2]	[-]	[MW]	[$\frac{kUSD}{a}$]
CASE A	0.5	-	0.0	166.8	6.0	2700.0	294.9
	1	-	0.0	184.7	6.0	2700.0	296.2
CASE B	0.5	-	0.0	210.1	6.0	2700.0	295.3
	1	-	0.0	167.5	6.0	2700.0	293.2
CASE C	0.5	50.0	435.0	402.7	8.0	2700.0	306.7
	1	50.0	435.0	402.7	8.0	2700.0	310.0
CASE D	0.5	-	0.0	390.0	7.0	3113.6	348.3
	1	-	0.0	380.3	7.0	3106.2	347.8

Table 4.3. Indirect: Main results of small example

problem has three hot process streams and three cold process streams that are in two different processes. Additionally, there is an option for one intermediate stream. The intermediate stream temperature is a variable that has a lower bound of 20 °C and an upper bound of 200 °C. T_{mapp} for all heat exchangers is 1. The number of stages is equal to two, although the optimal solution could be obtained with only one stage. This is calculated by minimizing only the utilities, i.e., multiplying the area and number of unit costs by zero in the objective function. Then the model is solved by steadily increasing the number of stages until the consumption of utilities does not increase anymore. Using this approach the number of stages is only one. Because in this example the calculation time is not a limiting factor, two stages are used. The cost coefficient for the indirect heat exchangers, $UNITC_A$, is varied from 0.5 to 1. The following four different cases are calculated.

1. Case A: Heat exchange between processes only allowed directly between process streams (normal heat exchanger network).

2. Case B: No restrictions on heat transfer

3. Case C: Direct heat exchange not allowed between process streams in different processes

4. Case D: Heat exchange not allowed between different processes at all

Discussion of the results of Example 1

The main results of all cases are shown in Table 4.3. As can be seen from the results, using indirect heat exchanging with intermediate streams is beneficial only if direct heat transfer between streams in different processes is restricted or forbidden for some reason. The results are logical indicating that the model is working robustly and correctly. In Case A, which is a normal heat exchanger network (no indirect heat transfer allowed), the total annual cost of the network should not be dependent on the value $UNITC_A$. In Case B, the total cost should increase with increasing $UNITC_A$ if indirect heat transfer occurs. But if no indirect heat transfer occurs, the values should not be dependent on $UNITC_A$. The total cost should be equally good or better in Case B compared to Case A. In Case C the total cost should be equally big or bigger than in Case B and the total cost should increase with increasing values of $UNITC_A$. In Case D the effect of increasing $UNITC_A$ on the total annual costs should be nonexistent and the total cost is equally big or bigger than in Case C. All the previous conclusions can be seen in the results shown in Table 4.3.

Because the model is non-convex, and the solvers used can only provide locally optimal solutions to non-convex problems, some minor illogicality can be seen in the results, but the major trends are logical indicating that the model is robust.

The final flowsheets of all cases with $UNITC_A = 0.5$ are shown in Publication I. The flowsheets are drawn with HeVi [67]. Because the software was originally meant for heat exchanger networks that do not have intermediate streams, an intermediate stream has to be presented as two streams, a hot intermediate stream (h4INT) and a cold intermediate stream (c4INT), although actually these two streams are the same stream.

4.1.2 Indirect: Example 2

Stream	TIN [°C]	TOUT [°C]	FCp [$\frac{kW}{°C}$]	Process	H [$\frac{kW}{m^2 \cdot °C}$]
H1	250	120	300	1	1
H2	500	120	250	2	1
H3	120	119	15000	3	1
H4	200	30	200	3	1
C1	165	220	500	1	1
C2	139	500	150	2	1
C3	20	250	100	2	1
C4	110	160	250	3	1
C5	200	201	25000	3	1
HU	1000	550	-	-	0.1
CU	5	6	-	-	1

Plant lifetime 7 years
Interest rate 8.0 (%/a)
Annuity factor 0.192072 (-)
HEX cost, streams in the same process (direct) [$] $= 8600 + 670 \cdot A^{0.83}$ (A in m^2)
HEX cost, streams in diff. processes (direct) [$] $= 2 * 8600 + 670 \cdot A^{0.83}$ (A in m^2)
HEX cost, streams in diff. processes (indirect) [$] $= UNITC_A * 2 * 8600 + 670 \cdot A^{0.83}$ (A in m^2)
Annual Hot Utility cost [$\$/kW \cdot a$] $= 100$
Annual Cold Utility cost [$\$/kW \cdot a$] $= 10$
H for hot and cold intermediate streams [$\frac{kW}{m^2 \cdot °C}$] $= 5$

Table 4.4. Process data for Example 2 (Indirect).

CASE	$UNITC_A$ [$-$]	T_{ha} [$°C$]	Int. str Q [kW]	Area [m^2]	Unit [-]	HU [MW]	Total cost [$\frac{kUSD}{a}$]
CASE A	0.5	-,-	0.0	18589.3	13.0	3751.0	1472.7
	1	-,-	0.0	18589.3	13.0	3751.0	1472.7
CASE B	0.5	-,-	0.0	18270.8	13.0	3552.5	1467.2
	1	-,-	0.0	18270.8	13.0	3552.5	1467.2
CASE C	0.5	181.3, 300.0	28500.0	17177.8	16.0	6315.3	1765.8
	1	181.3, 300.0	28482.1	17165.4	16.0	6341.6	1775.1
CASE D	0.5	-,-	0.0	12029.3	11.0	27460.1	3864.9
	1	-,-	0.0	12029.3	11.0	27460.1	3864.9

Table 4.5. Indirect: Main results of Example 2

The second example is taken from Ahmad and Hui [4], but the cost parameters are obtained from Kralj et al. [48]. The data are shown in Table

4.4.

There is an option for two intermediate streams and the process streams are grouped according to Ahmad and Hui [4]. For the first possible intermediate stream the temperatures have a lower bound of 40 °C and an upper bound of 300 °C. The second possible intermediate stream has a lower bound of 300 °C and upper bound of 500 °C. T_{mapp} for all heat exchangers is 1. the number of stages is equal to three. The same four different cases as were presented in Section 4.1.1 are calculated here.

Discussion of the results of Example 2

The main results are shown in Table 4.5. As can be seen from the results, the usage of intermediate streams is beneficial only if direct heat transfer between streams in different processes is restricted or forbidden for some reason. The model reacts reasonably logically. The only illogicality occurs in Case B, where the total costs should be the same as in Case A if indirect heat transfer is not used. If indirect heat transfer is used, the total cost of Case B should be less than or equal to Case A.

The final flowsheets of all cases with $UNITC_A = 0.5$ are shown in Publication I.

4.2 Results of examples solved with SingBilevelII

SingBilevelII was used to calculate three examples found in the literature. Additionally the same examples were calculated with the Synheat-model. The reason for this comparison is that both use the same superstructure. In this way the differences in the results are caused by algorithmic or methodological differences not differences in the modelling approach. The same initial values and bounds were used for both methods. The main results, i.e., the total annual cost and solution time of all three examples are given in Figure 4.1.

4.2.1 Example 1 of SingBilevelII

Example 1 was originally presented by Linnhoff and Ahmad [56]. The input data are given in Table 4.6, the detailed results are in Tables 4.7 and 4.8, and the final flowsheet obtained with two groups in Figure 4.2. Altogether, two major iterations were calculated, although the first iteration provided the best result. As can be seen from the results, there are two

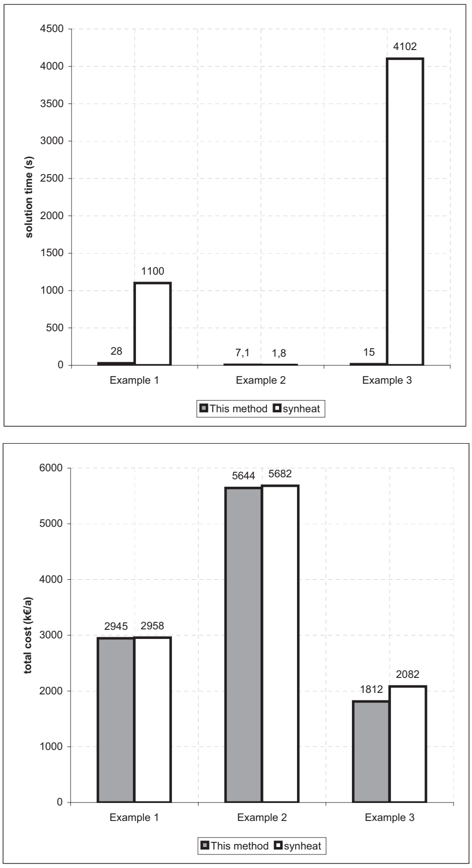

Figure 4.1. SingBilevelII: The main results of the three examples

groups (Group 1: H1, H4, C1, C3, C5 and Group 2: H2, H3, C2, C4) and the solution time for the method that is presented is notably less compared to the basic Synheat method for this example. The total annual cost is also slightly better with the presented method compared to the basic Synheat method, 2.945 and 2.958, M$/year respectively. Other researchers, for example Pettersson [71], Khorasany and Fesanghary [46], Lewin [51], and X. Luo and Fieg [88] have reported slightly better total annual costs, but they used different approaches or superstructures which might be better for this specific HENS problem. X. Luo and Fieg [88] also provide a list of results obtained also from other researchers. According to X. Luo and Fieg [88] the best known total cost is 2.922 M$/year obtained with their approach, although their list is missing Pettersson [71], who reported a total annual cost of 2.905 M$/year using his method.

Stream	TIN [$^\circ$C]	TOUT [$^\circ$C]	FCp [$\frac{kW}{^\circ C}$]	H [$\frac{W}{m^2 \cdot ^\circ C}$]
H1	327	40	100	0.50
H2	220	160	160	0.40
H3	220	60	60	0.14
H4	160	45	400	0.30
C1	100	300	100	0.35
C2	35	164	70	0.70
C3	85	138	350	0.50
C4	60	170	60	0.14
C5	140	300	200	0.60
HU	330	250	-	0.50
CU	15	30	-	0.50

Annual cost of HEX $[USD/a] = 2000 + 70 \cdot A^{0.8}$ (A in m^2)

Annual Hot Utility cost $[USD/kW \cdot a] = 60$

Annual Cold Utility cost $[USD/kW \cdot a] = 6$

Table 4.6. Process data for Example 1

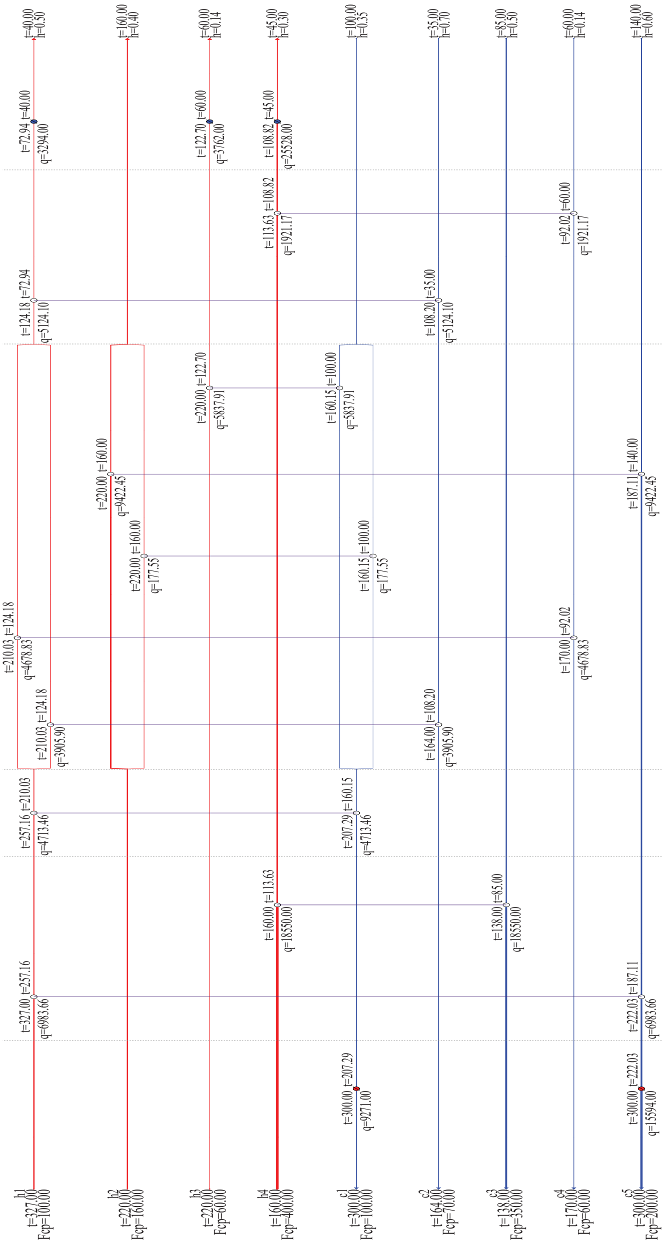

Figure 4.2. Flowsheet of Example 1 obtained with SingBilevelI (2 groups)

Stream	Reference value (USD/a)	Group
H1	72323.2	1
H2	18163.5	2
H3	60945.8	2
H4	251439.8	1
C1	91004.8	1
C2	11439.7	2
C3	29153.7	1
C4	24196.5	2
C5	133267.5	1
Aggregate stream parameter	Group 1	Group2
trhin	327.0	220.0
trhout	40.0	60.0
frh	260.3	120.0
hrh	0.203	0.245
trcin	85.0	35.0
trcout	300.0	170.0
frc	328.1	115.8
hrc	0.467	0.227

Table 4.7. Results of *Submodel-1* and *Submodel-2* for Example 1.

	This method: 2 groups	Synheat
Stages	4	4
T_{mapp}	14.5	14.5
Solution time [s]	28.08	1100.0
Total Area [m^2]	17532.7	18162.3
Units [-]	15.0	14.0
Hot Utility [MW]	24.9	24.4
Cold Utility [MW]	32.6	32.1
Total cost [k€/a]	2944.7	2957.6

Table 4.8. SingBilevelII: Results for Example 1

4.2.2 Example 2 of SingBilevelII

Example 2 is taken from Khorasany and Fesanghary [46]. The input data are given in Table 4.9, the detailed results are in Tables 4.10, and 4.11 and the final flowsheet obtained with two groups is in Figure 4.3. In the two groups streams H1, H4, H5, C3 and C4 are in group 1 and streams H2, H3, H6, C1, and C2 are in group 2. Three major iterations were solved although the optimum value was reached in the first iteration. As can be seen from the results, the solution time for SingBilevelII is comparable with the basic Synheat method for this example, which was solved very fast with both approaches. The reason for this might be that the problem had no fixed unit cost. The total annual costs are comparable with each other for both calculations (5644.0 and 5681.9 k$/year), although SingBilevelII gave a slightly better result. The result of SingBilevelII is slightly better if compared with the results presented in Khorasany and Fesanghary [46]. In this example it seems that, possibly because of the lack of fixed unit costs of heat exchangers, the superstructure used in the presented method and in the Synheat-model is competitive. Khorasany and Fesanghary [46] gives a list of detailed results of some researchers who have solved this problem. According to Khorasany and Fesanghary [46], the best known total cost is 5662.4 k$/year obtained with their approach, which is slightly worse than the result obtained with SingBilevelII.

Stream	TIN [$^\circ$C]	TOUT [$^\circ$C]	FCp [$\frac{kW}{^\circ C}$]	H [$\frac{W}{m^2 \cdot ^\circ C}$]
H1	85	45	156.3	0.05
H2	120	40	50.0	0.05
H3	125	35	23.9	0.05
H4	56	46	1250.0	0.05
H5	90	86	1500.0	0.05
H6	225	75	50.0	0.05
C1	40	55	466.7	0.05
C2	55	65	600.0	0.05
C3	65	165	180.0	0.05
C4	10	170	81.3	0.05
HU	200	198	-	0.05
CU	15	20	-	0.05

Annual cost of HEX $[USD/a] = 60 \cdot A^{1.0}$ (A in m^2)
Annual Hot Utility cost $[USD/kW \cdot a] = 100$
Annual Cold Utility cost $[USD/kW \cdot a] = 15$

Table 4.9. Process data for Example 2

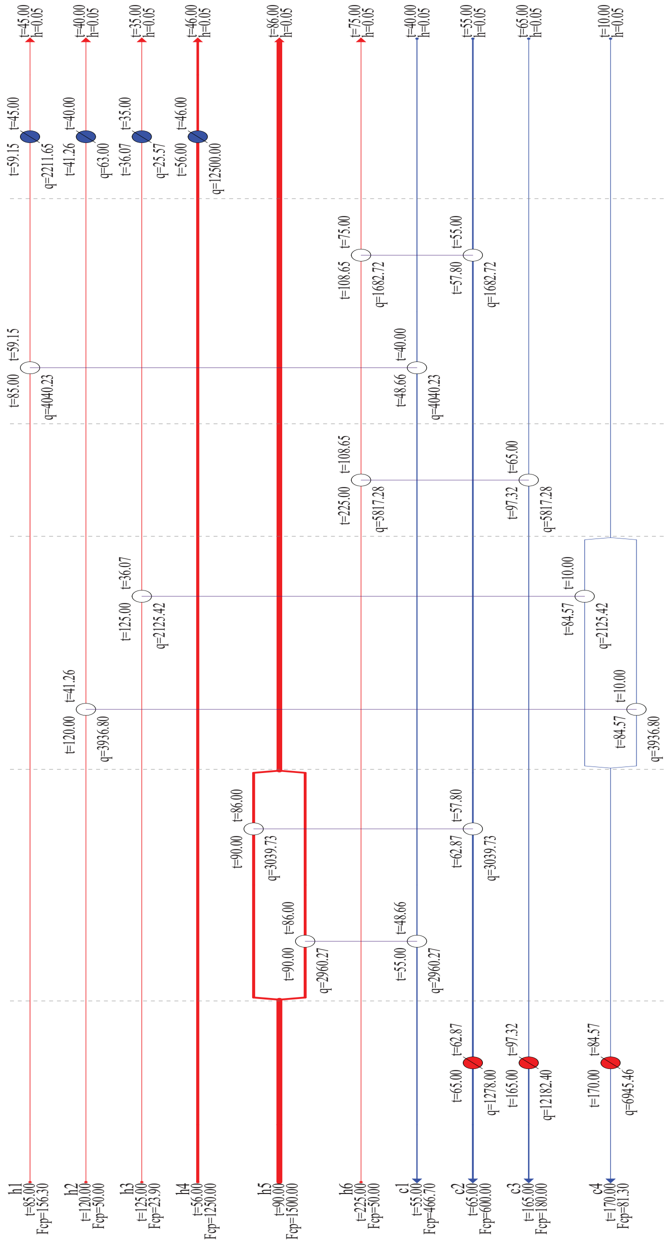

Figure 4.3. SingBilevelII: Flowsheet of Example 2 (2 groups)

Stream	Reference value (USD/a)	Group
H1	331432.7	1
H2	177230.8	2
H3	100467.4	2
H4	897190.2	1
H5	204258.7	1
H6	152408.6	2
C1	110967.1	2
C2	103625.7	2
C3	587874.8	1
C4	361333.5	1
Aggregate stream parameter	Group 1	Group2
trhin	90.0	225.0
trhout	50.5	35.0
frh	626.2	71.8
hrh	0.034	0.045
trcin	10.0	40.0
trcout	193.8	520.0
frc	328.1	115.8
hrc	0.042	0.049

Table 4.10. SingBilvelII: Results of *Submodel-1* and *Submodel-2* for Example 2.

	This method: 2 groups	Synheat
Stages	4	4
T_{mapp}	6	6
Solution time [s]	7.1	1.8
Total Area [m^2]	56356.8	56818.3
Units [-]	14.0	15.0
Hot Utility [MW]	20.4	20.5
Cold Utility [MW]	14.8	14.9
Total cost [k€/a]	5644.0	5681.9

Table 4.11. SingBilevelII: Results for Example 2

4.2.3 Example 3 SingBilevelII

Example 3 is taken from X. Luo and Fieg [88]. The input data are given in Table 4.12, the detailed results are in Tables 4.13 and 4.14, and the final flowsheet obtained with two groups is in Figure 4.4. Differently to SingBilevelII, the Synheat model used $T_{mapp} = 15\,^{\circ}\mathrm{C}$, because it was unable to solve the problem with values greater than $T_{mapp} = 15\,^{\circ}\mathrm{C}$. As can be seen from the results, there are two groups (G1:H3, H5, H6, H7, H8, C1, C2, C3, C5, C6, and G2: H1, H2, H4, H9, H10, C4, C7, C8, C9, and C10); three major iterations were solved, although the optimum value was reached in the first iteration and the total annual costs are better with SingBilevelII compared with the basic Synheat model (1811.9 and 2082.4 k$/year respectively). The solution time is clearly shorter, too. The total annual cost given by X. Luo and Fieg [88] is 1753.3 k$/year obtained by their method, which is slightly better than the one obtained with SingBilevelII. For this example their approach can be considered better, especially because they were able to find good results quite early in the calculations in their stochastic method and with decent solution times. On the other hand, it can be hard to find the correct parameters needed in their method.

4.2.4 SingBilvelII: Discussion

The proposed method SingBilevelII method can solve medium-sized HENS problems, providing solutions that are equally good with the Synheat model, which uses the same superstructure and assumptions. This conclusion can be drawn according to the three small to medium-sized HENS problems both methods were tested on. In general this should also occur with less computational effort, at least for larger problems, as was indicated by two of the example problems used in this work. The proposed method is a more complex model than the Synheat model, but for a normal user of these methods only basic stream and cost data need to be given and hence the user does not have to see the complex steps and models behind SingBilevelII. But for the mathematical solver, SingBilevelII is simpler than the Synheat method. Other methods that use different modeling approaches or superstructures can give better results, but not always, and not necessarily very robustly.

Regarding the proposed method, it is very important to build an aggre-

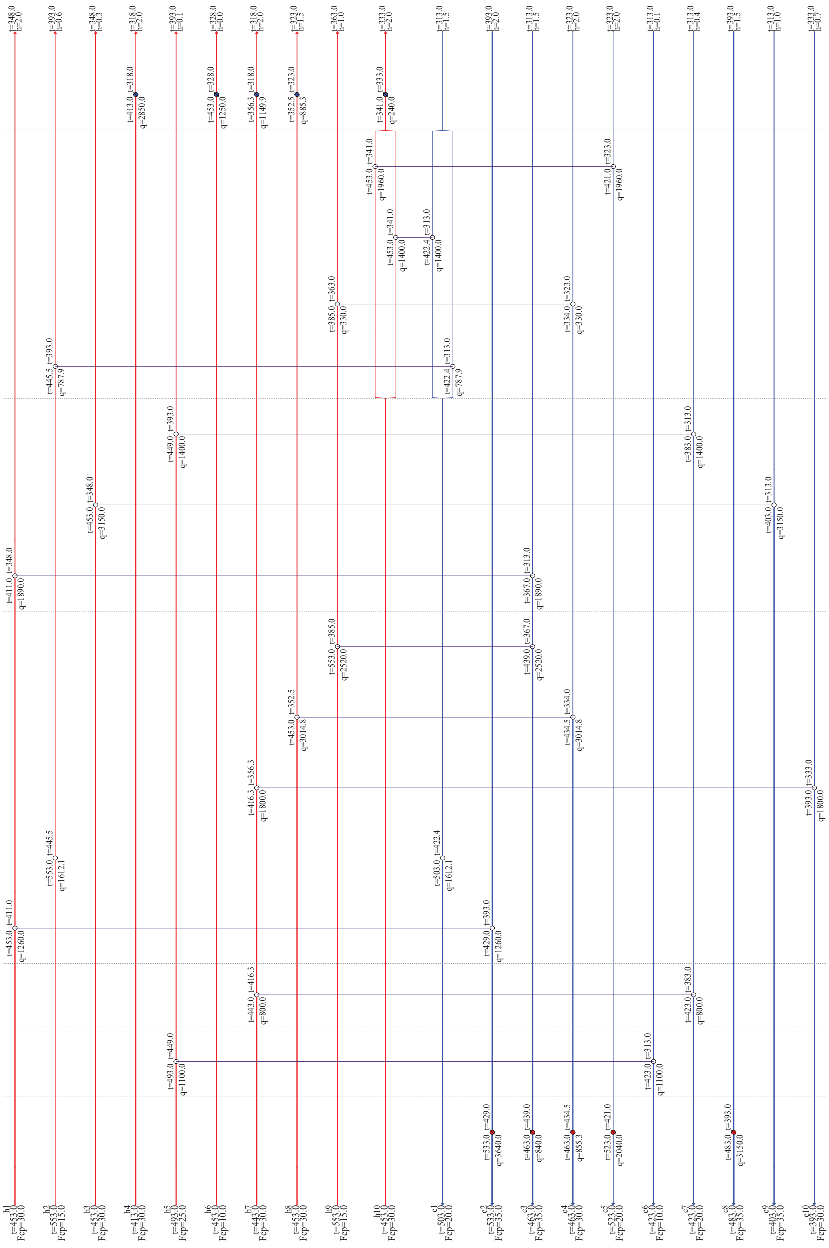

Figure 4.4. SingBilevelII: Flowsheet of Example 3 (2 groups)

Stream	TIN [$^\circ$C]	TOUT [$^\circ$C]	FCp [$\frac{kW}{^\circ C}$]	H [$\frac{W}{m^2 \cdot ^\circ C}$]
H1	453	348	30	2.00
H2	553	393	15	0.60
H3	453	348	30	0.30
H4	413	318	30	2.00
H5	493	393	25	0.08
H6	453	328	10	0.02
H7	443	318	30	2.00
H8	453	323	30	1.50
H9	553	363	15	1.00
H10	453	333	30	2.00
C1	313	503	20	1.50
C2	393	533	35	2.00
C3	313	463	35	1.50
C4	323	463	30	2.00
C5	323	523	20	2.00
C6	313	423	10	0.06
C7	313	423	20	0.40
C8	393	483	35	1.50
C9	313	403	35	1.00
C10	333	393	30	0.70
HU	598	598	-	1.00
CU	298	313	-	2.00

Annual cost of HEX $[USD/a] = 8000 + 800 \cdot A^{0.8}$ (A in m^2)

Annual Hot Utility cost $[USD/kW \cdot a] = 70$

Annual Cold Utility cost $[USD/kW \cdot a] = 10$

Table 4.12. Process data for Example 3

gate stream in such a way that its total annual cost equals to the total annual cost of the streams that the aggregate stream represents. On the other hand, the results of grouping the streams are not that important. Generally speaking, the grouping step affects the solution time, but the appropriate aggregate streams affect the quality of the results.

Stream	Reference value (USD/a)	Group
H1	14072.0	2
H2	13191.3	2
H3	41230.2	1
H4	20374.3	2
H5	65085.7	1
H6	181811.1	1
H7	22165.2	1
H8	23385.6	1
H9	12761.3	2
H10	17548.7	2
C1	14252.8	1
C2	21240.1	1
C3	16388.6	1
C4	12804.6	2
C5	14976.9	1
C6	28270.4	1
C7	13479.9	2
C8	13347.5	2
C9	11028.7	2
C10	8329.8	2
Aggregate Stream parameter	Group 1	Group2
trhin	493.0	553.0
trhout	376.6	393.0
frh	125.0	92.8
hrc	0.058	0.224
trcin	313.0	313.0
trcout	471.8	409.7
frc	120.0	150.0
hrc	0.209	0.201

Table 4.13. SingBilevelII: Results of *Submodel-1* and *Submodel-2* for Example 3.

4.3 Results of examples using the A–GAMS–NIMBUS-tool

The A–GAMS–NIMBUS-tool presented here has been used in solving two examples.

4.3.1 A–GAMS–NIMBUS-tool: Example 1

Example 1 is taken from Björk and Westerlund [13]. The stream data can be found in Table 4.15. The heat exchanger cost parameters for the example are shown in Table 4.16, even though they are not used in this case (but are used with the basic single-objective Synheat model for comparison). The number of stages is two and t_{map}, the minimum allowed approach temperature, is 0.1. Table 4.17 shows values of the objective functions in different NIMBUS iterations. First, the *nadir* and *ideal* objective values are calculated for all four objectives (*Units*, *Area*, *Hot Util-*

	This method: 2 groups	Synheat
Stages	5	5
T_{mapp}	18	15
Solution time [s]	14.5	4102.0
Total Area [m^2]	3004.7	4979.9
Units [-]	24.0	27.0
Hot Utility [MW]	10.5	9.4
Cold Utility [MW]	6.4	5.2
Total cost [k€/a]	1811.9	2082.4

Table 4.14. SingBilevelII: Results for Example 3

ity, and *Cold Utility*). With this information the initial solution is calculated and the values of the four objectives are shown to the DM. Next (iteration 2), the DM is asked to classify the objectives. In this case the DM allows the *Units* objective to increase from its current value of 6 to at most 7. The DM wants both of the objectives *Area* and *HU* to be in class $I^{<}$, and hence they should be minimized as much as possible. The fourth objective, *CU*, is in class $I^{\diamond}$ and can vary freely in this iteration and also in all the subsequent iterations. This is mainly because the DM understands from the calculations so far and from his previous knowledge of HENS that *CU* is very strongly coupled with the objective *HU*, and in this case, the DM decided that the objective *HU* is more important than *CU*. With this classification Model (3.3) is solved. As can be seen, the values of *Units*, *HU*, and *CU* are all quite close to their *ideal* values, but *Area* is quite far from its ideal value. For this reason, the DM decides to improve the value of the objective *Area* in the next iteration. In iteration 3 the objective *Units* should not increase from its current level, but the objective *HU* can increase to 2500. The objective *Area* should be minimized as much as possible. Once again Model 3.3 is optimized and the results are presented to the DM. This procedure continues until after iteration 5 the DM decides to stop the optimization procedure being pleased with the results.

Figure 4.5 shows the final flowsheet of example (1). As can be seen from the figure, only one stage is sufficient and no stream splits are needed. Additionally, three of the four process streams have an utility exchanger, indicating that the network is probably operationally flexible.

When Example 1 is solved with the original single-objective Synheat model, with the same parameters (number of stages allowed in the superstructure equal to two, t_{map} equal to 0.1 and with the same solvers) and with the cost parameters given in Table 4.16, the minimized total annual cost is equal to 429.4 kEuro. If this result is compared with the results of the final iteration shown in Table 4.17 obtained by using the A–GAMS–NIMBUS-tool, and using these values of the objective functions to calculate the total annual cost with the same cost parameters (Table 4.16) after the optimization, the total annual cost is 423.5 kEuro, which is slightly better than with the single-objective Synheat model. Although the reason for this might be the use of local solvers, it certainly gives a strong indication of the potential of the A–GAMS–NIMBUS-tool. It is important to note, that in the A–GAMS–NIMBUS tool the total annual cost was not optimized, but was calculated after the optimization with the values of the optimized objective functions. Additionally, if the cost parameters were to vary slightly, the final network obtained with the A–GAMS–NIMBUS-tool would not necessarily change, unless the DM wanted to change it.

Stream	T_{in} (°C)	T_{out} (°C)	Fc_p (KW/K)	h (kW/m^{2}K)
H1	180	75	30	0.15
H2	240	60	40	0.10
C1	40	230	35	0.20
C2	120	300	20	0.10
Hot Utility	325	325	-	2.00
Cold Utility	25	40	-	0.50

Table 4.15. A–GAMS–NIMBUS-tool: Stream data for Example 1 taken from Table 1 in [13].

USD/a	USD/(a m^2)		USD/(a kW)
$CF_{ij} = 15000$	$C_{ij} = 30$	$\beta_{ij} = 0.8$	$CCU = 10$
$CF_{i,CU} = 15000$	$C_{i,CU} = 30$	$\beta_{i,CU} = 0.8$	$CHU = 110$
$CF_{i,HU} = 15000$	$C_{i,HU} = 60$	$\beta_{i,HU} = 0.8$	

Table 4.16. A–GAMS–NIMBUS-tool: Heat exchanger and utility cost parameters for Example 1.

4.3.2 Example 2 of A–GAMS–NIMBUS-tool

Example 2 is taken from Linnhoff and Ahmad [56]. The stream data for the example are the same as Example 1 of Chapter 4.2 and are given in Table 4.18. Altogether, four hot streams and five cold streams are present.

The cost parameters are equal for all the heat exchangers, namely $CF = 2000$ USD/a , $C = 70$ USD/(a m^2) and $\beta = 1.0$. The cold and hot

Iteration k	*Issue*	*Units [-]*	*Area* $[m^2]$	*HU [kW]*	*CU [kW]*
1(Init.)	Ideal	4	2385	1756	1856
	Nadir	9	426236	7100	7200
	Sol.	6	287728	5354	5454
2	Classes	$I^{\geq}$	$I^{<}$	$I^{<}$	$I^{\diamond}$
	Bounds	UP=7			
	Opt. values	7	15335	1919	2019
3	Classes	$I^{=}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$
	Bounds	FX=7		UP=2500	
	Opt. values	7	7478	2500	2600
4	Classes	$I^{\leq}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$
	Bounds	LO=5		UP=3000	
	Opt. values	5	5834	3000	3100
5	Classes	$I^{=}$	$I^{\geq}$	$I^{<}$	$I^{\diamond}$
	Bounds	FX=5	UP=8000		
	Opt. values	5	8000	2457	2557

Table 4.17. A–GAMS–NIMBUS-tool: Results of iterations of Example 1

utility costs are 6 USD/(a kW) and 60 USD/(a kW) respectively, although these are not needed for the interactive formulation. They are given here because these cost parameters are used in the basic single-objective Synheat model, whose results are compared to the ones obtained with the A–GAMS–NIMBUS-integration tool. Altogether, five stages are allowed in the superstructure and t_{map}, the minimum allowed approach temperature, is 1.

Table 4.19 shows the values of the objective functions in different NIMBUS iterations and Figure 4.6 shows the final flowsheet. In this case the

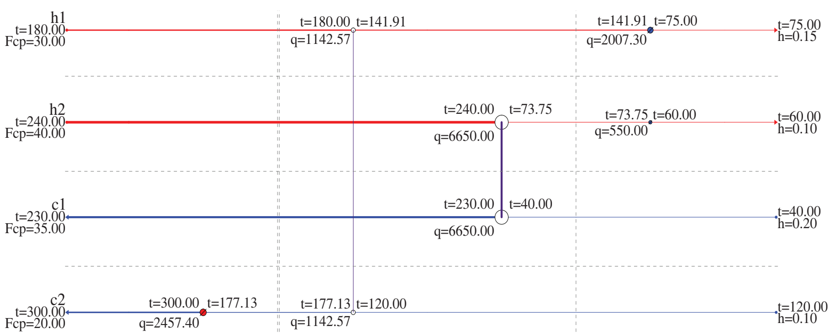

Figure 4.5. A–GAMS–NIMBUS-tool: Final flowsheet of Example 1

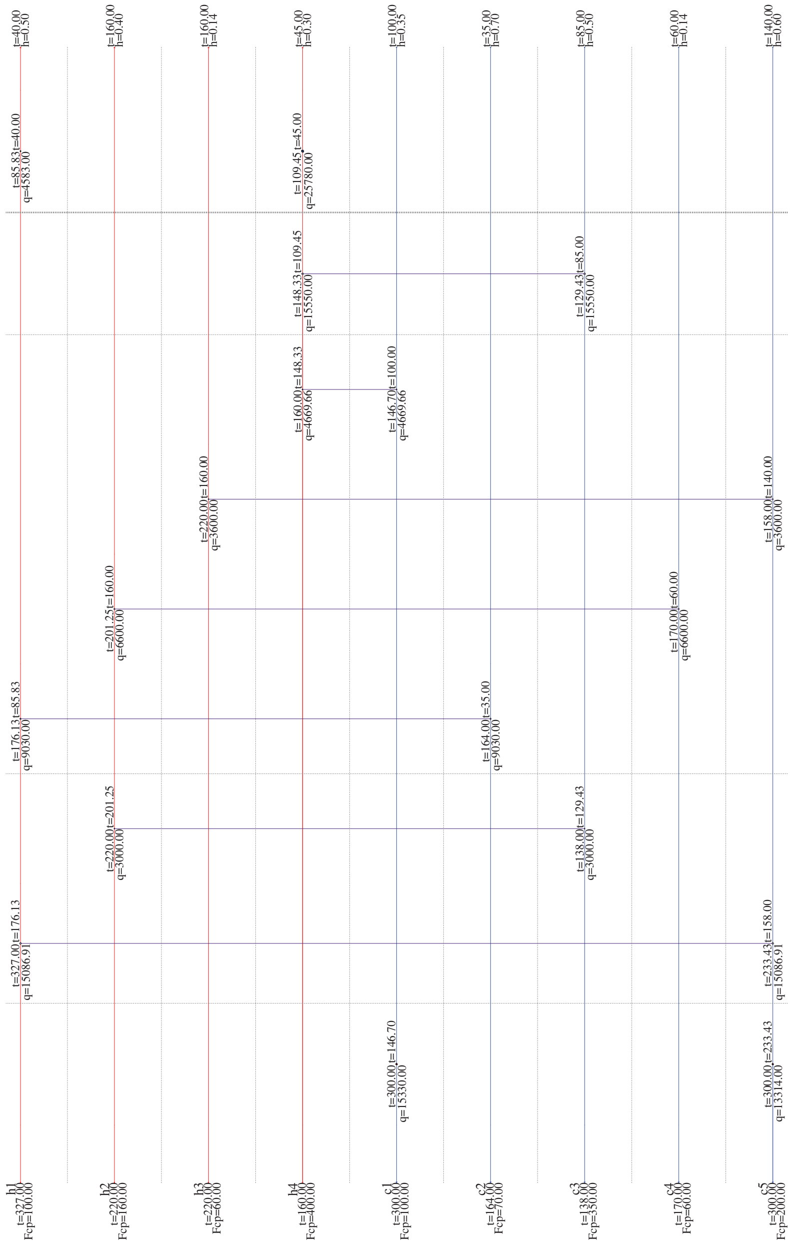

Figure 4.6. A–GAMS–NIMBUS-tool: Final flowsheet of Example 2

Stream	T_{in} (°C)	T_{out} (°C)	Fc_p (KW/K)	h (kW/m^{2}K)
H1	327	40	100	0.50
H2	220	160	160	0.40
H3	220	60	60	0.14
H4	160	45	400	0.30
C1	100	300	100	0.35
C2	35	164	70	0.70
C3	85	138	350	0.50
C4	60	170	60	0.14
C5	140	300	200	0.60
Hot Utility	330	250	-	0.50
Cold Utility	15	30	-	0.50

Table 4.18. A–GAMS–NIMBUS-tool:Stream data for Example 2 taken from [56].

Iteration k	*Issue*	*Units [-]*	*Area* $[m^2]$	*HU [kW]*	*CU [kW]*
1(Init.)	Ideal	9	9519	15300	17020
	Nadir	68	270946	54430	56150
	Sol.	14	36459	19332	20336
2	Classes	$I^{\leq}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$
	Bounds	LO=10		UP=27000	
	Opt. values	10	16722	27000	28720
3	Classes	$I^{\geq}$	$I^{\leq}$	$I^{\geq}$	$I^{\diamond}$
	Bounds	UP=11	LO=15000	UP=29000	
	Opt. values	11	15986	29000	30720
4	Classes	$I^{=}$	$I^{\geq}$	$I^{\leq}$	$I^{\diamond}$
	Bounds	UP=11	UP=16000	LO=27000	
	Opt. values	11	16000	28643	30363

Table 4.19. A–GAMS–NIMBUS-tool: Results of iterations of Example 2

DM was already happy with the results after four iterations. The final flowsheet needs only three stages and no stream splits are needed. Altogether, 11 heat exchangers, of which four are utility exchangers, are needed.

When example 2 is solved with the original single-objective Synheat model, with the same parameters (number of stages allowed in the superstructure equal to five, t_{map} equal to 1 and with the same solvers) and with the given cost parameters, the minimized total annual cost is equal to 4.4 MEuro. If this result is compared with the results of the final iteration shown in Table 4.19 obtained by using the A–GAMS–NIMBUS-tool, and using these values of the objective functions to calculate the total annual cost with the same cost parameters, after the optimization, the total annual cost is 3.0 MEuro, which is substantially better than with the single-objective Synheat model, indicating once again the potential of the presented A–GAMS–NIMBUS-tool, although it is also very clear, that the single-objective Synheat model was stuck at a very bad local solution.

4.4 Results of examples using MOBilevelI

MOBilevelI has been used in solving two examples found in the literature.

4.4.1 Example 1 using MOBilevelI

Example 1 is the same example as that used in Section 4.2. The input data are given in Table 4.6. There are three stages in the superstructure.

Iteration k	*Issue*	*Units [-]*	*Area* $[m^2]$	*HU [kW]*	*CU [kW]*	*Time [s]*
1(Init.)	Ideal	9.0	9811.5	16070.0	23790.0	
	Nadir	37.0	248835.2	67630.0	75350.0	
	Sol.	16.0	48175.0	41850.0	49570.0	4.7
2	Classes	$I^{\diamond}$	$I^{<}$	$I^{<}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	-	-	-	
	Initial Values	16.0	48175.0	41850.0	49570.0	
	Opt. values	16.0	29752.0	20371.4	28091.40	10.3
3	Classes	$I^{\leq}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$	
	Bounds/aspiration levels	14.0	-	25000	-	
	Initial values	16.0	29752.0	20371.4	49570.0	
	Opt. values	12.0	19799.2	25000.0	32720.0	21.6
4	Classes	$I^{\geq}$	$I^{\leq}$	$I^{<}$	$I^{\diamond}$	
	Bounds/aspiration levels	17.0	18000.0	25700.0	-	
	Initial values	12.0	19799.2	25000.0	32720.0	
	Opt. values	13.0	18399.5	25700.0	33420.0	11.9
5	Classes	$I^{\diamond}$	$I^{\geq}$	$I^{<}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	18500	-	-	
	Initial values	13.0	18399.5	25700.0	33420.0	
	Opt. values	14.0	18500.0	24599.7	32319.7	11.6
6	Classes	$I^{\diamond}$	$I^{\geq}$	$I^{<}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	19570.0	-	-	
	Initial values	12.0	19799.2	25000.0	32720.0	
	Opt. values	13.0	19200.0	23891.03	31611.03	8.2

Table 4.20. MOBilevelI: Results of iterations of Example 1

The results of the different major iterations are shown in Table 4.20 and the final flowsheet (major iteration 6) in Figure 4.7. As can be seen from the calculation procedure, in the second iteration the DM wanted to minimize both the area and the hot utilities, while the number of units and the cold utilities were not that important. This is because the DM, having experience in designing heat exchanger networks, knows that the main trade-off is between hot utility consumption and the heat exchanger area. Additionally, in most cases the cold utility and hot utility consumption correlate closely, and typically it is the hot utility that is worth more. In the third iteration the DM wanted to improve the area and was ready to impair the hot utility consumption. In the third iteration the DM also wanted to improve the number of units, but the cold utility could be freely varied. In the fourth iteration, a slight improvement for the area was still wanted, but in this iteration both the hot utility consumption and the number of units could be impaired slightly. The result of this iteration was interesting to the DM, but she/he wanted to vary this result slightly in the fifth iteration, where the area could be impaired slightly, while the hot utility consumption should be improved as much as possible. In the last iteration the DM wanted the same as in iteration 5, but now with increased willingness to impair the area objective. After this the DM decided, although the results from all of the last three iterations were acceptable, to choose the results from iteration 6 as the final heat exchanger network.

The final heat exchanger network is shown in Figure 4.7.

Interestingly, although the number of units could be varied freely in most major iterations, the changes from the starting solutions were small or non-existent. Whether this is truly optimal or the solution is stuck at a local optimum is not known.

Example 2 using MOBilevelI

Example 2 is taken from X. Luo and Fieg [88]. The input data are given in Table 4.12.

The results of the different major iterations are shown in Table 4.21. There are four stages in the superstructure. As can be seen from the results, altogether six major iterations were used before the DM was satisfied with the results. As the final solution the DM chose the solution of the fifth iteration. This final heat exchanger network is shown in Figure 4.8. As can be seen from the calculation procedure, in the second iteration the DM wanted to minimize both the area and hot utilities, while the number of units and the cold utilities were not that important. In the third iteration the DM wanted to improve the total area of heat exchangers while letting the hot utility consumption increase. In iteration 4 the DM wanted to improve the hot utility consumption while letting the total area increase slightly. In the fifth iteration it was the area that was minimized as much as possible, while the hot utility consumption could be increased to 10550 kW. The DM was satisfied with the solution of the fifth iteration, but wanted to test this solution so that both the hot utility consumption and total area could be increased slightly. This could then

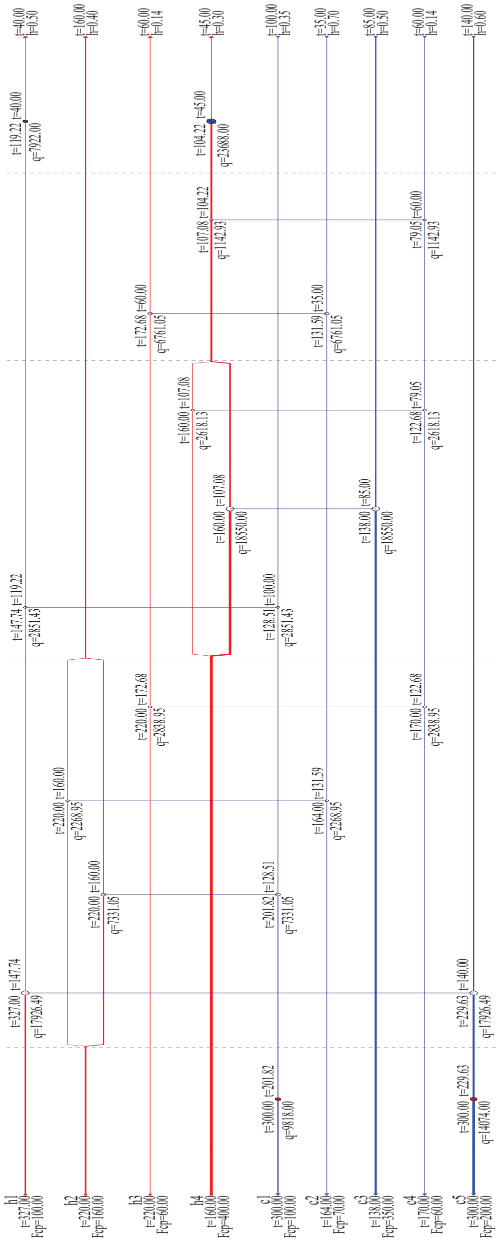

Figure 4.7. MOBilevelI: The final heat exchanger network of Example 1

give the possibility of reducing the number of units. Although this solution was also satisfying for the DM, the DM chose the fifth iteration as the final solution.

Iteration k	*Issue*	*Units [-]*	*Area* $[m^2]$	*HU [kW]*	*CU [kW]*	*Time [s]*
1(Init.)	Ideal	18.0	2026.3	4655.0 505.0		
	Nadir	84.0	236995.9	27883.6	23733.6	
	Sol.	24.0	119510.8	16269.3	12119.3	12.1
2	Classes	$I^{\diamond}$	$I^{<}$	$I^{<}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	-	-	-	
	Initial Values	24.0	119510.8	16269.3	12119.3	
	Opt. values	36.0	7965.1	5242.1	12850.0	145.3
3	Classes	$I^{\diamond}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	-	12000	-	
	Initial Values	36.0	7965.1	5242.1	12850.0	
	Opt. values	29.0	4132.3	12000.0	7850.0	47.3
4	Classes	$I^{\diamond}$	$I^{\geq}$	$I^{\leq}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	5000	10500	-	
	Initial Values	29.0	4132.3	12000.0	7850.0	
	Opt. values	27.0	5000.0	10500.0	6350.0	63.2
5	Classes	$I^{\diamond}$	$I^{<}$	$I^{\geq}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	-	10550.0	-	
	Initial Values	27.0	5000.0	10500.0	6350.0	
	Opt. values	30.0	3233.2	10550.0	6400.0	83.9
6	Classes	$I^{\diamond}$	$I^{\geq}$	$I^{\geq}$	$I^{\diamond}$	
	Bounds/aspiration levels	-	3250.0	12000.0	-	
	Initial Values	30.0	3233.2	10550.0	6400.0	
	Opt. values	28.0	3250.3	12000.0	7850.0	69.0

Table 4.21. MOBilevelI: Results of iterations of Example 2

4.4.2 MOBilevelI: Discussion of the results

There are some important remarks to make about the method that is presented and the results obtained for the two examples. One issue is the fact that typically single-objective solvers providing only locally optimal solutions are used, as was the case with the examples. This can cause confusion to the DM, because the results do not always fully follow the classifications of the DM because there are only locally Pareto optimal solutions. Global optimization algorithms and techniques would solve this problem, but unfortunately global optimization methods are currently computationally too demanding for industrial-sized heat exchanger networks.

Another important remark is that there are differences in the solutions provided by the two scalarization functions. In the examples studied, the scalarization of Equation (3.5) almost always provides feasible solutions, although sometimes it is clear that the solutions are only locally Pareto optimal. The scalarization function of Equation (3.4), on the other hand, has sometimes problems finding a feasible solution either for *Submodel-3* or for *Submodel-4*. When it finds a solution, the solutions are almost always good. The reason for the problems observed in finding feasible so-

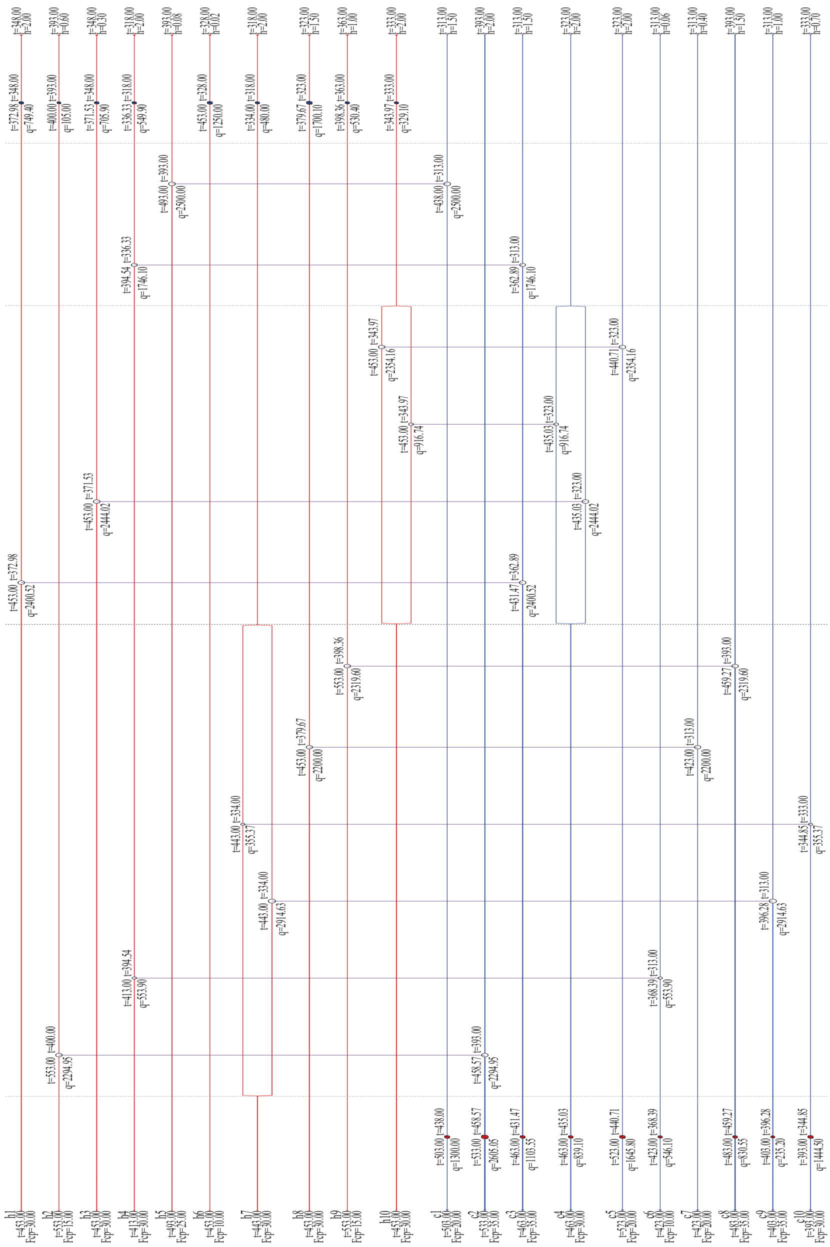

Figure 4.8. MOBilevelI: The final heat exchanger network of Example 2

lutions is related to the different natures of the scalarization functions. Equation (3.4) tries to obey the classification provided as closely as possible with upper bounds, whereas Equation (3.5) has a more relaxed approach. It can find a feasible solution where the desires of the DM cannot be fully respected (if it is impossible to obey all those desires). The strict upper bounds used in Equation (3.4) direct the search to infeasible areas. After the classification, upper bounds are given to the values of the different objectives that are based on the classification and the current value of the objective functions. These values are based on *Submodel-4*, which is similar to *Submodel-3* but still different from it. Occasionally, it can happen that the starting point is not appropriate for *Submodel-3* and hence no solution is found.

Because no decompositions are used in solving the ideal number of heat exchanger matches, the solution time for this part is considerable and even unacceptably long, at least for the problems with many streams. For this reason it is helpful to use a different number of stages for this part of the methodology, use the bilevel decomposition approach to solve this problem or even try to approximate this value with some other approach.

Another potential problem is that if the ideal solution is not actually ideal (because of local solvers), the search space is restricted in all solutions. However, this seems not to be a problem in HENS if the Synheat based superstructure is applied.

5. Conclusions and contribution of the thesis and future work

This thesis presents new approaches for designing Heat Exchanger Networks. Although a lot of different methods have been presented for the HENS problem in recent decades, there is still a need for new methods that are able to solve the HENS problem in such a way that the computational effort is reduced without the quality of the results being affected. One reason for this is that energy efficiency in the process industry has to be increased in a cost-efficient way, providing a need for more detailed HENS models and the broader integration of HENS into larger process synthesis problems. The need for computationally more efficient methods stems from the fact that the HENS problem has been proven to be NP-hard and hence a polynomially converging general algorithm probably does not exist. For this reason HENS methods that provide good approximate solutions with reasonable computational requirements are important. The objective of this thesis has been to aid in achieving this goal, *i.e.*, to present new HENS methods that try to be computationally efficient without the quality of the results being affected. In most of the methods of this thesis the approach to achieving this objective has been to group the process streams, either artificially or according to the reality that in most real industrial processes the process streams are already grouped, depending on the process section that the process streams belong to. Another approach in some of the methods has been to use an interactive multiobjective optimization method to achieve the objective of providing good results without too great a computational burden.

One of the methods, called Indirect, is a new MINLP model for HENS that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes. In this case the process streams are grouped according to the process section they belong to in an industrial process. The multiobjective approach used is the traditional weighted sum approach, where the weights are the annual costs of heat exchangers, the annual cost of heat exchanger area and the annual costs of both hot and cold utilities. In addition to optimizing a normal heat exchanger network, the model provides the possibility of analyzing and optimizing the option of using intermediate streams as a medium to transfer heat between different process sections. Intermediate streams are used in order to reduce the number of transfer units between processes, because of the physical distance between the processes and for operational flexibility reasons. A modified version of the Synheat model is used as the superstructure-generating approach in the model. The main conclusions regarding the model are that it works logically and that considering the possibility of using intermediate streams for indirect heat transfer can sometimes be beneficial, especially if direct heat transfer between streams in different processes is restricted or forbidden or the cost of direct heat exchanging between different processes is very high.

Another method presented in this thesis is the bilevel optimization method for simultaneous HENS called SingBilevelII. The objective of the method is to efficiently and robustly provide an optimized heat exchanger network where all the elements of the objective function are optimized simultaneously. The efficiency of the method means that HENS problems should be solved with as little computational effort as possible without the quality of the results being affected. The overall method has four steps or submodels that are combined into an overall method. The multi-objective approach used is the traditional weighted sum approach, where the weights are the annual costs of heat exchangers, the annual cost of heat exchanger area, and the annual costs of both hot and cold utilities. SingBilevelII can solve medium-sized HENS problems, providing solutions that are equally good as or better than the ones obtained with the Synheat model, which uses the same superstructure and assumptions. This conclusion can be reached according to the three small to medium-sized HENS problems both methods were tested on. In general this should also occur with less computational effort, at least for larger problems, as was indicated by two of the example problems. The proposed method is more complex to model than the Synheat model, although for a normal user of these methods only basic stream and cost data need to be given and hence the user does not see the complex steps and models behind the method that is presented. But importantly, for the actual solvers, this method is simpler than the basic Synheat model. The main conclusion concerning the method is that it can solve at least medium-sized HENS problems in a computationally more efficient way than existing methods that have the same superstructure and with equally good results.

The third new simultaneous HENS approach presented in this thesis, called the A-GAMS-NIMBUS-tool, uses interactive multiobjective optimization for the HENS problem. The benefit of using interactive multiobjective optimization is that it is possible to find the solution that best satisfies the DM without too great a cognitive or computational load, and, compared to the traditional approach of using fixed weights for the objectives, all the possible Pareto optimal solutions can be found. Another benefit is that the cost information of the different objectives is not that important, although it can be used. Another benefit is that the DM is in control of the design procedure, as in pinch technology. Additionally, the method that is presented introduced a tool called the A-GAMS-NIMBUS-tool, which implements a simplified version of the interactive multiobjective optimization method NIMBUS into the General Algebraic Modeling System, GAMS, so that GAMS can solve multiobjective optimization problems without using weighting factors. This tool can easily be applied to fields outside HENS.

The fourth new simultaneous HENS approach, called MOBilevelI, combines the interactive multiobjective optimization method with the bilevel optimization method. The objective of this approach is to combine the benefits of both methods so that HENS problems can be solved in a computationally efficient way and so all the Pareto optimal solutions can be found. According to the results of the example problems, this objective can be achieved.

As a new tool, but not a new method, Publication VI of this thesis introduces a new visualization tool for heat exchanger networks that are optimized using the Synheat superstructure.

5.1 Contribution of the thesis

The main contribution of this thesis is new HENS methods that are designed to be computationally efficient without the quality of the results being affected. According to the results of the examples that were used to test the methods, this goal is also achieved.

In the new MINLP model for HENS that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes, the key novelty is the possibility of simultaneous energy and capital cost optimization for heat transfer between processes. Although many methods found in the open literature consider heat transfer between different process sections, in none of them is this achieved by simultaneous synthesis, at least in situations where direct heat transfer between streams in the same processes and both direct and indirect heat transfer between process streams in different processes are included. In some of these methods this is accomplished sequentially with pinch analysis-based tools, but this can easily lead to the best solutions being cut off.

The innovation in the simultaneous HENS method that uses bilevel optimization, stream data grouping, and the aggregation of streams is in the overall procedure of the method. Although the grouping of streams, aggregate streams, and even bilevel optimization are used in other methods, they are not combined in a manner that provides results as competitive as the one presented in this thesis. This is especially true regarding the objective of the overall method, i.e., to simplify HENS problems so that they can be solved in a computationally efficient way while getting good results.

Previously, interactive multiobjective optimization has not been applied to HENS problems. With interactive multiobjective optimization there is a possibility of finding the network that best satisfies the DM without too great a cognitive or computational load, and compared to the traditional approach of using fixed weights for the objectives, all the possible (local) Pareto optimal solutions can be found. Another benefit is that the cost information of the different objectives is not necessarily needed, although it can be used, making the optimized network less sensitive to changes in economic parameters. Additionally, the A-GAMS-NIMBUS-tool can be seen as a beneficial contribution to applying interactive multiobjective optimization in fields outside HENS too.

The method that combines the A-GAMS-NIMBUS-tool and the bilevel HENS method combines two innovative methods, providing a means to solve HENS problems in a computationally efficient way and one in which all the Pareto optimal solutions can be found.

Overall, the contribution of this thesis is a group of novel, robust, and easy-to-use methods that provide the designer of heat exchanger networks with a means to design cost- and energy-efficient heat exchanger networks that also work in a computationally efficient way.

Overall the contribution of this thesis is a group of novel, robust and easy-to-use methods that provide the designer of heat exchanger networks a means to design cost- and energy efficient heat exchanger networks also computationally efficiently.

5.2 Future work

The methods presented in this thesis form a solid basis for further work and developments in the field of HENS.

In the MINLP model for HENS that allows simultaneous heat integration directly between streams in the same process and both directly and indirectly between streams in different processes, there should be a possibility of the intermediate streams not being isothermal, but of their temperature changing when they are heated or cooled. The superstructure should be improved so that different integration possibilities, such as the integration of the utility system, different heat pump technologies etc., could be embedded into the superstructure. This would, on the other hand, increase the size of the problem and might reduce the robustness of the model. A very direct continuation of this thesis would be to apply the interactive multiobjective A-GAMS-NIMBUS-tool to solve the different objectives of the model without the traditional weighting method. In order to solve bigger problems the bilevel approach could be used in solving the model, either with or without the interactive A-GAMS-NIMBUS-tool. This would certainly need adjustments to the model, but these adjustments would be reasonably straightforward.

The bilevel optimization approach could be used to solve more detailed HENS problems (varying specific heat capacities, pressure drop considerations etc.) and to apply the method in retrofit situations. Certainly, more detailed models would be needed and probably a different approach to the grouping of process streams would be needed, especially in the retrofit situation, but there is no major barrier in view that hinders this possibility. In this way the benefit of the computational efficiency of the bilevel approach would be efficiently utilized.

Another interesting possibility would be to utilize the bilevel optimization method in other fields of process synthesis that are outside HENS. In most cases this would call for the readjustment of the method, but in some cases, such as in the synthesis of mass exchanger networks, the method should be more or less directly applicable.

A more theoretical further study related to the bilevel optimization method could be the analysis of the convergence properties of the bilevel method. It would be very interesting would be to know in which situations the bilevel method is able to reach the global optimum if global optimum algorithms are used. An important question to study is whether *Submodel-3* can be forced to be a very tight underestimation of *Submodel-4*. Another issue that should be studied is why the results obtained with the bilevel approach (when using local solvers) are typically better than the results obtained without the bilevel approach. It would be logical if these were equally good (sometimes better, sometimes worse), but now they are almost always better. Does the smaller problem size help the GAMS parameters in finding better solutions?

The A-GAMS-NIMBUS-tool should be developed to take into account all the developments of all the current and future features of the IND-NIMBUS software. These issues include, for example, the possibility of using different scalarizing functions and calculating the intermediate points between two Pareto optimal solutions. That is, when new Multicriteria Decision Making methods are implemented into the IND-NIMBUS software framework, those methods would also be available for models implemented with the A-GAMS-NIMBUS-tool. Currently, in the A-GAMS-NIMBUS-tool the NIMBUS method is implemented as part of the GAMS model, with the NIMBUS-specific GAMS equations being added to the original GAMS model by hand, combining the GAMS model and the NIMBUS implementation into a single GAMS-NIMBUS model. A more general approach, in which the implementation of the NIMBUS method is contained in the initialization and scalarization models, and separated from the original GAMS model, would be beneficial. The HEVI visualization tool could also be directly integrated into the A-GAMS-NIMBUS-tool so that optimized networks would be presented to the DM automatically.

A direct continuation of the A-GAMS-NIMBUS-tool in HENS would be to model flexibility issues and consider flexibility as an additional objective function that should be maximized.

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Errata

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New methods for Heat Exchanger Network Synthesis are presented in this thesis. Heat Exchanger Network Synthesis is a key step in designing energy-efficient industrial processes in a cost-efficient way. This synthesis problem has also been proven to be a hard to solve with exponentially increasing solution time with linearly increasing problem size. In this thesis bilevel optimization based on grouping of process streams is used as a new approach to improve the computational efficiency. The multiobjective synthesis problem is solved with the bilevel approach together with a traditional weighting method and with an interactive multiobjective optimization method. The benefit of using interactive multiobjective optimization is that it is possible to find the solution that best satisfies the Decision Maker without too much cognitive or computational load, and all possible Pareto optimal solutions can be found.

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