TKK Dissertations 27
Espoo 2006

A SYSTEMATIC PROCEDURE FOR ANALYSIS AND DESIGN OF ENERGY SYSTEMS

Doctoral Dissertation

Tor-Martin Tveit

Helsinki University of Technology
Department of Mechanical Engineering
Laboratory of Energy Engineering and Environmental Protection

TKK Dissertations 27
Espoo 2006

A SYSTEMATIC PROCEDURE FOR ANALYSIS AND DESIGN OF ENERGY SYSTEMS

Doctoral Dissertation

Tor-Martin Tveit

Dissertation for the degree of Doctor of Science in Technology to be presented with due permission of the Department of Mechanical Engineering for public examination and debate in Auditorium K216 at Helsinki University of Technology (Espoo, Finland) on the 28th of April, 2006, at 12 noon.

Helsinki University of Technology
Department of Mechanical Engineering
Laboratory of Energy Engineering and Environmental Protection

Teknillinen korkeakoulu
Konetekniikan osasto
Energiatekniikan ja ympäristönsuojelun laboratorio

Distribution:
Helsinki University of Technology
Department of Mechanical Engineering
Laboratory of Energy Engineering and Environmental Protection
P.O. Box 4400
FI - 02015 TKK
FINLAND
URL: http://eny.tkk.fi/
Tel. +358-9-451 3631
Fax +358-9-451 3418
E-mail: tor-martin.tveit@tkk.fi

ISBN 951-22-8096-5
ISBN 951-22-8097-3 (PDF)
ISSN 1795-2239
ISSN 1795-4584 (PDF)
URL: http://lib.tkk.fi/Diss/2006/isbn9512280973/

TKK-DISS-2110

Picaset Oy
Helsinki 2006

HELSINKI UNIVERSITY OF TECHNOLOGY P. O. BOX 1000, FI-02015 TKK http://www.tkk.fi	ABSTRACT OF DOCTORAL DISSERTATION

Author Tor-Martin Tveit

Name of the dissertation

A systematic procedure for analysis and design of energy systems

Date of manuscript March 15, 2006	Date of the dissertation April 28, 2006
☐ Monograph	☒ Article dissertation (summary + original articles)

Department	Mechanical Engineering
Laboratory	Energy Engineering and Environmental Protection
Field of research	Energy technology
Opponent(s)	Daniel Favrat, professor, and Frank Pettersson, D.Sc.(Tech)
Supervisor	Carl-Johan Fogelholm, professor
(Instructor)	Juha Aaltola, D.Sc.(Tech.)

Abstract

The new re-regulated markets for electricity, stricter environmental policies and regulations, especially regarding greenhouse gases, form a new operating environment for energy systems. The new environment requires systems that are cost-efficient and have more efficient utilisation of energy with a low negative environmental impact. This can only be achieved with efficient tools for analysing and designing current and future energy systems.

The objective of this work is to present a systematic procedure for analysis and design of energy systems. The procedure utilises simulation modelling, experimental design and regression models and mathematical programming. The procedure is able to simplify large problems so that they can be efficiently solved, but still preserve sufficient amount of details so that the objective of the analysis or design can be fulfilled. The main advantage of the methodology is that it can reduce the size of the problems in a way that is more flexible than existing methodologies using mathematical programming. This is important, since it can efficiently reduce the complexity of the problem, and can thus be used to analyse and design complex energy systems with respect to several objectives. In this respect the procedure can be seen as a valuable addition to the existing methodologies.

Keywords Energy systems, MINLP modelling, Simulation, Experimental Design

ISBN (printed) 951-22-8096-5	ISSN (printed) ISSN 1795-2239
ISBN (pdf) 951-22-8097-3	ISSN (pdf) ISSN 1795-4584
ISBN (others)	Number of pages 68 p. + app. 74 p.

Publisher Energy Engineering and Environmental Protection

Print distribution Energy Engineering and Environmental Protection

☒ The dissertation can be read at http://lib.tkk.fi/Diss/2006/isbn9512280973/

Preface

The work presented in this dissertation has been carried out at the Department of Mechanical Engineering at Helsinki University of Technology during the years of 1999–2005.

My warmest thanks to all my colleagues, who have made our workplace such a nice place to work.

Finally, my sincere thanks to my supervisor, professor Carl-Johan Fogelholm for giving me the opportunity to work in such a good environment and for giving me the opportunity to write this dissertation.

Helsinki, March 2006

Tor-Martin Tveit

Contents

List of Publications

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

I Tveit, T.-M. *"A simulation model of a sulphuric acid production process as an integrated part of an energy system"*, Simulation Modelling Practice and Theory, 11, 7–8 (2003), 585–596.

II Tveit, T.-M. *"A methodology for improving large scale thermal energy systems"*, Applied Thermal Engineering, 24, 4 (2004), 515–524.

III Tveit, T.-M., Aaltola, J., Laukkanen, T., Laihanen, M., Fogelholm, C.-J. *"A framework for local and regional energy system integration between industry and municipalities - Case study UPM-Kymmene Kaukas"*, Energy, In Press.

IV Tveit, T.-M. *"Experimental design methods and flowsheet synthesis of energy systems"*, Applied Thermal Engineering, 25, 2–3 (2005), 283–293.

V Tveit, T.-M., and Fogelholm C.-J. *"Multi-period steam turbine network optimisation, Part I: Simulation based regression models and an evolutionary algorithm for finding D-optimal designs"*, Applied Thermal Engineering, 26, 10 (2006), 993–1000.

VI Tveit, T.-M., and Fogelholm C.-J. *"Multi-period steam turbine network optimisation, Part II: Development of a multi-period MINLP model of a utility system"*, Applied Thermal Engineering, In Press.

Author's contribution

In *Publication I* the development of a simulation model for a sulphuric acid plant using a commercial software package for power plant process simulation is presented. The development of realistic simulation models is a crucial part of the methodology presented in this dissertation. The results of the work presented in Publication I show that it is possible to use inexpensive but powerful power plant process simulation software to model a common chemical process as a part of a large energy system.

Publication II indicates how factorial designs can be applied in the synthesis of energy systems. In addition the outline of a methodology combining *simulation*, *experimental design* and *mathematical programming* is presented.

In *Publication III* a large framework for energy integration examination between municipalities and the industry is applied to a case. The publication focuses on two methodologies, of which one is the methodology presented in *Publication II*. The results of the publication show that the methodology can be successfully applied together with other methodologies. The author was responsible for the application of the methodology presented in *Publication II*, the overall interaction of the methodologies and the presentation of the final results of the study.

Publication IV is a presentation of how to utilise established methods from the field of experimental design in the flowsheet synthesis of energy systems. The work is based on the work presented in Publication II. The results of the publications show that the methodology has a good potential for reducing the optimisation problem and subsequently for solving more complex problems than the traditional methods are able to solve. This is shown through an example that is solved both by using a MINLP model, where all the units are modelled in detail, and by using the new

methodology.

In *Publication V* a method for finding regression models for steam turbine networks using a simulation model and an evolutionary algorithm for finding D-optimal designs is presented. There are two major problems that are addressed in Publication V. First, the evolutionary algorithm for finding D-optimal design is applied to try to solve the problem of which values to simulate to generate the data for the regression model. Second, a theoretical model of steam turbine performance is used to model the feasible operation of the steam turbine. The author was responsible for almost all aspects of the publication. Co-author Fogelholm contributed by commenting the work.

In *Publication VI* the method presented in Publication V is used to develop and solve a multi-period optimisation model of a steam turbine network in a utility system. This demonstrates how the methodology can be applied when building a multi-period optimisation model to estimate and evaluate how changes to the processes will affect the utility system. The author was responsible for almost all aspects of the publication. Co-author Fogelholm contributed by commenting the work.

List of Abbreviations

CHP	combined heat and power
lad	least absolute deviation
LP	linear programming
lsq	least squares
NLP	nonlinear programming
MILP	mixed integer linear programming
MINLP	mixed integer nonlinear programming
SQP	successive quadratic programming

List of Figures

1 Introduction

A well functioning modern society is dependent on a reliable and cost-efficient supply of useful energy. The economic and environmental impacts of energy systems make it important to continously improve and develop these systems. In addition to the indirect effects on the economy, energy systems also have a significant directly economic importance. For example, in Finland, the annual average value of imported fuels and electricity between 2000 and 2003 was 2340 million euros [58]. In the years 1991 to 2001 the investments directly connected to energy conversion in Finland amounted to an annual average of 783 million euros [58]. The environmental impact of energy systems is also considerable. Carbon dioxide, sulfur dioxide and nitrogen dioxide are some examples of important emissions from energy systems that affect the environment. Carbon dioxide is by far the most important greenhouse gas, and the total carbon dioxide emissions in Finland in 2002 were 82 million ton (approximately 2 % of total EU emissions). From the 82 million ton, 37 million ton was from power plants and boilers and 11 million ton was from the combustion of fossil fuels in industrial processes. Sulphur dioxide and nitrogen dioxide in the atmosphere can lead to acid precipitation (acid rain) [9]. Sulfur dioxide inhalation is also a cause for damage to the upper respiratory tract and to lung tissue [29]. The emissions of sulfur dioxide and nitrogen dioxide from power plants and boilers in Finland in 2002 were 54000 ton and 69400 ton respectively. The nitrogen dioxide emission from power plants and boilers where approximately 33 % of the total nitrogen dioxide emissions in Finland, and the similar figure for sulfur dioxide is 63 % [58].

The new re-regulated[1] markets for electricity, together with stricter environmental policies and regulations, especially regarding greenhouse gases, form an operating environment for energy systems that require a more efficient utilisation of energy with a low negative environmental impact. This can only be achieved with efficient

[1]The term "*de-regulation*" is often used for the change of regulation regime. However, as the markets are still regulated, the regime change is more accurately described as a *re-regulation*.

tools for analysing and designing energy systems.

1.1 Energy system analysis and design

In the context of the work presented in this dissertation, an *energy system* is a collection of connected units that participate in the conversion and utilisation of energy, and that is the subject of the analysis or design. The system has a *system boundary* that defines the inputs and outputs of the system. An example of an energy system is a CHP plant, where the system is a boiler with pre- and superheaters, additional heat exchangers, turbines, generators, flue gas filters and scrubbers, pumps and a feed water tank. The inputs to the system is fuel, air and cooling water, while the output is heat (as either hot water or steam), flue gases and electricity. Another example of an energy system is the one studied in Publication III, which is a combined pulp and paper plant together with a municipal district heating network.

The analysis of an energy system can be to identify the performance of an existing system in relation to a certain criterion, or to evaluate how changes to the system or surroundings will affect the performance of the system.

The design of an energy system is the process of defining the desired inputs and outputs, and selecting the corresponding process cycles and the process topology. The topology consists of the selected equipment and connections between the equipment. Flowsheet synthesis is an important part of the design process of energy systems. Flowsheet synthesis can be defined as the process of generating many alternative conceptual flowsheets, often in the form of a superstructure, and selecting the topology and system parameters that give rise to the flowsheet that is optimal for a given objective or objectives. As the resulting flowsheets are conceptual, flowsheet synthesis precedes the detailed design, where the accurate and detailed description of the construction of the equipment is elaborated. A brief overview of approaches to

the design of chemical processes can be found in the work by Westerberg [74]. If the objective of the design is to modify an existing system, the design process is referred to as retrofit design.

The process of analysing and designing an optimal energy system is not inconsequential, and there are many challenges related to the process.

1.2 Challenges related to energy system analysis and design

There are numerous requirements and objectives for an energy system. The system should for instance be efficient, have a low or no negative environmental impact, be safe, have high controllability, be easy to maintain and be profitable from an economic perspective. The modelling of only one of these requirements can be challenging, and it is not feasible to include all of these objectives simultaneously in a comprehensive analysis or design process. An important challenge related to energy system design is to choose the correct measure of performance and the most relevant objectives to include in the analysis or design process. In addition to this, the level of detail must be chosen, *i.e.* to which level of accuracy should the objectives and subsequent constraints be analysed or modelled? The analysis and design in this work has been limited to the efficiency of a system[2] and economic performance. However, the procedure developed is not limited to these objectives, and can be applied to any of the requirements and objectives mentioned.

At present it is almost impossible to analyse or design a system without a proper model of the system in question. Many of the challenges related to energy system analysis and design are related to the modelling of the system. For instance, the modelling of the behaviour of units and subsystems comprising the system, the

[2]The environmental impact of the system is indirectly included, since the efficiency of the system has a significant effect on the environmental impact.

modelling of thermodynamic properties, choice and interactions of parameters, the structural complexity of energy systems and uncertainties, are all important factors that add to the overall complexity of the analysis or design process. The degree of complexity the factors add is also dependent upon which methodology is chosen, as different methodologies handle the complexities differently.

There is no methodology available that can comprehensively take into account all the factors relevant to the analysis and design of energy systems. The existing methodologies are specialised methods designed to efficiently handle a selection of the factors relevant to the analysis or design process. The systematic procedure suggested in this work uses a combination of simulation, regression modelling, experimental design and mathematical programming. Mathematical programming is used to find the best solutions in relation to the objectives of the analysis or design. The regression models based on simulation modelling are used together with an experimental design to simplify the optimisation model, while maintaining a realistic model of the energy system.

1.3 Objectives of this work

The objective of this dissertation is to present a systematic procedure for finding optimal solutions to the design or redesign of energy systems. The procedure utilises simulation modelling, experimental design, regression models and mathematical programming. The main advantage of the methodology is that it will present a novel approach to reducing the size of the problems that is more flexible than the existing methodologies using mathematical programming.

1.4 Overview of this work

In Section 2 an introduction to the available techniques, an overview of methodologies and approaches relevant to this work are presented. In Section 3 the objective and the scientific significance of this dissertation is presented in more detail. Section 4 presents the systematic procedure suggested in this work. In addition to the presentation of the procedure, the objective of the section is to summarise and connect the work in Publications I to VI that together with the overview comprise the dissertation. The conclusions and significance of the work are summarised in Section 5 together with recommendations for further work.

2 Literature review

In this section an overview of methodologies and approaches to the design and analysis of energy systems is presented. Readers who are familiar with mathematical programming, simulation of energy systems and experimental design, might wish to pass directly to Sections 2.1, 2.2.4 and 2.4.1, where the work that is particularly relevant to this dissertation is presented.

There are traditionally two approaches to the design and synthesis of energy systems, namely the *thermodynamic approach* and the approach using *optimisation* (deterministic or stochastic). This is a loose division, as the approaches are often mixed.

2.1 Thermodynamic approaches to the design of energy systems

Nishio et al. [48] developed a thermodynamic approach to steam-power system design. The approach uses heuristic rules and is limited to steam cycles. Chou and Shih [14] proposed a similar procedure, and developed a systematic procedure for the design of plant utility systems. The procedure helps in finding the configuration with the maximum allowable overall thermal efficiency. The procedure could also include gas turbine cycles.

El-Sayed and Evans [21] introduced the concept of *thermoeconomics*, where the inefficiencies of a system are given a cost. All the costs of the process streams are related to the exergetic value of the stream. Thermoeconomics expands the traditional thermodynamic analysis by including economic considerations. However, the methodology is not designed to handle other multi-objectives (*e.g.* reduction of the negative environmental impact of a process).

An important branch of the thermodynamic approach focuses on the entropy generation of the energy systems. Two closely related concepts are the *entropy generation minimisation* and *exergy loss minimisation*. The term *exergy* was first suggested by Rant [51]. The two concepts are introduced in the books by Kotas [36], Szargut et al. [59] and Bejan [3]. The purpose is to identify and minimise the irreversibilities of the processes. Some additions and refinements to the approaches relevant to this work is the use of the exergy approach to minimise costs by Tsatsaronis and Moran [64] and the identification of avoidable and unavoidable exergy losses by Tsatsaronis and Park [65].

Pinch analysis is a methodology that can be used to design a heat exchanger network with a fixed utility consumption. The fact that the minimum utility requirements for a heat exchanger network can be calculated only from the stream information and the minimum temperature difference in the heat exchangers was noted by Hohmann [30], although similar concepts had already been explored for blast furnaces in 1927 by Reichardt [52]. The concept was independently discovered by Linnhoff [41] and his group at UMIST who developed the concept into a tool for industrial processes. Pinch analysis can also be used to integrate new equipment and processes to a system, *e.g.* as in the work by Townsend and Linnhoff [62, 63].

A common problem with the thermodynamic approach is the lack of handling trade-offs. Even if, as mentioned above, several adaptations to the thermodynamic methods have been made to address this problem in special cases, the general problem still remains. In an attempt to overcome this, *Optimisation* has been applied.

2.2 Optimisation approaches to the design energy systems

Optimisation can be divided into deterministic optimisation (mathematical programming) and stochastic optimisation (*e.g.* evolutionary algorithms and simulated

annealing). In the following sections a brief introduction to the concepts of optimisation, as well as the use of the concepts in the design and analysis of energy systems is presented.

2.2.1 Mathematical programming

In the following section a brief introduction to different aspects of mathematical programming is given. In Section 2.2.4 applications of mathematical programming for the design and synthesis of energy systems are presented.

Mathematical programming, or deterministic optimisation, deals with the problem of optimising an objective function. A general formulation of a mathematical programming problem is given in Equation 2.1.

$$\min f(\mathbf{x}) \quad \text{subject to} \quad \mathbf{x} \in X \tag{2.1}$$

where $X \subseteq \mathcal{R}^n$ is the constraint set, $\mathbf{x}$ is an n-dimensional vector, and $f : \mathcal{R}^n \rightarrow \mathcal{R}^1$ is the objective function defined on X.

A point $\mathbf{x} \in X$ is called a feasible solution to the problem. If $\mathbf{x}^* \in X$ and there exists an ϵ-neighbourhood $N_\epsilon(\mathbf{x}^*)$ around $\mathbf{x}^*$ so that $f(\mathbf{x}^*) \leq f(\mathbf{x}) \; \forall \; x \in X \cap N_\epsilon(\mathbf{x}^*)$, then $\mathbf{x}^*$ is called a *local* optimal solution[2]. If $\mathbf{x}^* \in X$ and $f(\mathbf{x}^*) \leq f(\mathbf{x}) \; \forall \; \mathbf{x} \in X$, $\mathbf{x}^*$ is called a *global* optimal solution. The problem in Equation 2.1 can also be stated as a maximisation problem, by noting that both $\max f(\mathbf{x})$ and $\min -f(\mathbf{x})$ has the same optimal solution $\mathbf{x}^*$.

Mathematical programming problems are often divided into different classes, depending on their characteristics and structure. An important characteristic of the mathematical programming problem is whether the problem is *constrained* or *unconstrained*. If f is a function defined on $\mathcal{R}^n$ and $\mathbf{x}$ is an n-dimensional vector, an

unconstrained problem can be formulated as [4]:

$$\min f(\mathbf{x}) \quad \text{subject to } \mathbf{x} \in \mathcal{R}^n \tag{2.2}$$

which is similar to the problem in Equation 2.1, but where the constraint set X has been replaced by the n-dimensional Euclidean space. For constrained problems, X can be defined by a set of constraints, as shown in Equation 2.3

$$X = \left\{ \mathbf{x} : \begin{cases} h_i(\mathbf{x}) = 0, & i \in \{1, 2, \ldots, m\} \\ g_i(\mathbf{x}) \leq 0, & i \in \{1, 2, \ldots, l\} \end{cases} \right\} \tag{2.3}$$

where h_i and g_i are functions defined on $\mathcal{R}^n$. The functions h_i and g_i are often referred to respectively, as equality and inequality constraints.

Another important characteristic is whether the problem is *continuous* or *discrete*. A continuous problem is a problem where the constraint set X is infinite and has a 'continuous' character [4], and a discrete problem is simply a problem that is not continuous. An important sub-class of the discrete problems are problems where some of the decision variables must take only integer variables, so-called *integer programming* problems. In the case where the problem contains both continuous and integer variables, the problems are called *mixed integer* problems. Consider the general formulation of a constrained mixed integer problem shown in Equation 2.4.

$$\min f(\mathbf{x}, \mathbf{y}) \quad \text{subject to} \begin{cases} h_i(\mathbf{x}, \mathbf{y}) = 0, & i \in \{1, 2, \ldots, m\} \\ g_i(\mathbf{x}, \mathbf{y}) \leq 0, & i \in \{1, 2, \ldots, l\} \\ \mathbf{x} \in X \subseteq \mathcal{R}^n, \ \mathbf{y} \in Y \subseteq \mathcal{Z}^m & \end{cases} \tag{2.4}$$

where $\mathcal{Z}^m$ is the m-dimensional set of integers. If the objective function, f, or at least one of the constraints is nonlinear, the problem is called a *mixed-integer nonlinear programming* (MINLP) problem. Similarly, in the special case where the objective function and all the constraints are linear, the problem is called a *mixed integer linear programming* (MILP) problem. If the problem only contains continuous variables

(*i.e.* $Y = \emptyset$), the mixed-integer nonlinear programming problem is reduced to a *nonlinear programming* (NLP) problem and the mixed integer linear programming problem is similarly reduced to a *linear programming* (LP) problem.

There is no efficient algorithm for solving problems of all classes, but many specialised algorithms have been developed. It is often convenient to consider the classification of the mathematical programming problems into LP, NLP, MILP and MINLP, in relation to the algorithms used to solve the problems. For LP problems, and to some extent MILP problems, powerful algorithms exist to solve practical problems to a deterministic global optimum. For the nonlinear problems, algorithms exist to solve both NLP and MINLP problems to global optimal solutions (for instance Floudas [23], Ryoo and Sahinidis [54], and Smith and Pantelides [56]). A good overview of global optimisation can be found in the work by Floudas et al. [24]. However, the most efficient algorithms require that the functions are convex in order to guarantee a global optimal solution. For nonconvex problems with multimodal objective function or nonconvex feasible region, the classical nonlinear programming algorithms will terminate with a solution, which is strongly dependent on the starting point [60]. Unfortunately, these problems are common in the design and synthesis of energy systems. This means that for models regarding the design and synthesis of energy systems, the nonlinearities (in particular the nonconvex) and combinatorial complexities that are included in the models in order to arrive at a realistic model of the system, will often result in models for which no efficient optimisation algorithm exist. One alternative is to improve the algorithms, or to reformulate the models (*e.g.* convexifying the problem). Another approach is to avoid the problems by trying to reduce the problem.

The choice of algorithm is strongly dependent on the problem formulation and characteristics. To be able to solve a problem efficiently, it is therefore important to choose the correct algorithm based on an analysis of the optimisation model. For instance, two well known solvers for MINLP problems, SBB [1] and DICOPT [12]

work very differently, and generally DICOPT should perform better in problems where the combinatorial complexity is dominant, while SBB should perform better in problems with difficult nonlinearities and few discrete variables [70]. However, in practice it is difficult, even for the relatively simple linear programming problems, to predict how easy it is to solve a mathematical programming problem. For instance, even though Dantzig's *simplex method* for linear programming has a very poor theoretical worst-case behaviour, it has proven to be very successful in solving practical linear programming problems [55]. The difficulty to predict how difficult (or easy) different problems are to solve in practice is even more acute for MILP, NLP and MINLP problems.

2.2.2 Multiobjective optimisation

It is common when working with design of energy systems to have situations with more than one objective. For instance, the objectives can simultaneously be to minimise the negative environmental impact of the process, maximise the profit and to maximise the safety of the process. These problems are referred to as *multiobjective mathematical programming* problems. Equation 2.5 shows how a multiobjective optimisation problem can be formulated mathematically.

$$\min f_j(\mathbf{x}) \; \forall j \in \{1, 2, \ldots, k\} \quad \text{subject to} \quad \mathbf{x} \in X \tag{2.5}$$

where we have $k \geq 2$ objective functions $f_j : \mathcal{R}^n \rightarrow \mathcal{R}^1$. The *feasible objective region* Z, is the image of the feasible region (*i.e.* $Z = \mathbf{f}(X) \subset \mathcal{R}^k$). The elements of Z are called *objective vectors*. The objective vectors are denoted by $\mathbf{f}(\mathbf{x})$ or by $\mathbf{z} = [z_1, z_2, \ldots, z_k]^T$, where $z_j = f_j(\mathbf{x}) \; \forall j \in \{1, 2, \ldots, k\}$ [45]. The ideal optimal solution to Equation 2.5 would be a vector $\mathbf{z}^{**}$, that is simultaneously the optimal solution for each of the objective functions subject to the constraints. The vector $\mathbf{z}^{**}$ is often called the *ideal objective vector*. However, the ideal objective vector is often infeasible and unobtainable due to conflicts between the objectives. This

means that a different criterion for optimality must be defined. A common way of defining optimality is the *Pareto optimality*. The Pareto optimality can be defined as follows:

Definition 1. *An objective vector* $\mathbf{z}^* \in Z$ *is Pareto optimal in the absence of another objective vector* $\mathbf{z} \in Z$ *such that* $z_j \leq z_j^* \; \forall j \in \{1, 2, \ldots, k\}$*, and* $z_j < z_j^*$ *for at least one index* j*. (*Adapted from [45]*)*

There are usually many Pareto optimal solutions, and the set of Pareto optimal solutions is referred to as the *Pareto optimal set*. Pareto optimal solutions are mathematically equal, and a *decision maker* is needed to select the preferred solution. In the case of the decision maker being able to state the preferences before the solution process, *a priori* methods can be applied. Examples of a priori methods are the *value function method*, *lexicographical ordering* and *goal programming*. *A posteriori* methods generate the whole (or parts) of the Pareto optimal set, and present the generated set to the decision maker. The decision maker then selects the preferred solution. Two examples of a posteriori methods are the *weighting method* and the *ϵ-constraint method*. In this work the *ϵ-constraint method* is applied to multiobjective optimisation problems. The *ϵ-constraint method* was used since it is easy to implement into the mathematical programming modelling language used in this work. In this method, first presented by Heimes et al. [28], one objective function is chosen to be optimised. The remaining objective functions are transformed into constraints with an upper bound, ϵ. A formulation of the problem is presented in Equation 2.6

$$\min f_l(\mathbf{x}), \quad l \in \{1, 2, \ldots, k\}$$
$$\text{subject to} \begin{cases} f_j(\mathbf{x}) \leq \epsilon_j, & \forall j \in \{1, 2, \ldots, k\} \backslash l \\ \mathbf{x} \in X \end{cases} \tag{2.6}$$

A slight modification of Equation 2.6 was applied in this work. The inequality constraints of the objectives that were transformed into constraints were changed into equality constraints. This alternative formulation was proposed by Lin [40].

2.2.3 Evolutionary algorithms and simulated annealing

As a good complement to traditional mathematical programming, *evolutionary algorithms* have become popular tools for finding optimal solutions. The most basic forms of these algorithms are genetic algorithms and evolution strategies. A good overview of evolutionary algorithms is given in the paper by Whitley [75]. Genetic algorithms were first developed by Holland [31], while evolution strategies were developed by Rechenberg and Schwefel (see the article by Beyer and Schwefel [5]).

Genetic algorithms are search algorithms that are based on the analogy of improving a population of solutions through modifying their gene pool. Genetic algorithms emphasise the use of a 'genotype' that is decoded and evaluated. These genotypes are often simple data structures. The genotypes are modified using two forms of genetic modification, crossover and mutation. *Evolution strategies* are in many ways similar to genetic algorithms, but they have fewer constrains on the representation of the problem. The mutation also changes according to a statistical distribution. Evolution strategies are generally applied to real-valued representations of optimisation problems, and tend to emphasise mutation over crossover.

Simulated annealing is an optimisation strategy for combinatorial optimisation problems that uses the analogy of finding the low-temperature state of a system (Kirkpatrick et al. [35]). The strategy starts with a point, x, and an objective value, $f(x)$. An effective temperature, T, for the optimisation problem is introduced. A new point, x', is chosen at random from a distribution. If the new point improves the objective, the new point is accepted. In the case where the new point does not improve the objective, the point is accepted with probability distribution $p(T, x', x)$. This is done because only accepting a new point that improves the objective is similar to extremely rapid quenching, where the result is likely to be metastable with only locally optimal structures. The strategy continues by gradually reducing the effective temperature (and thus the degrees of freedom) until no further improvement

to the objective is achieved.

2.2.4 Mathematical programming, evolutionary algorithms and simulated annealing for design of energy systems

Mathematical programming has been widely applied in the design of energy systems in particular and in process design in general. In their two articles, Biegler and Grossmann [7, 27] give a good overview of mathematical programming and their application to process design and process systems engineering. This section presents some of the previous work particularly relevant to this work.

Bruno et al. [11] developed a rigorous MINLP model for the synthesis of power plants. By using the formulations they suggested it is possible to solve larger synthesis problems of real plants. In their work Manninen and Zhu [43] took a different approach and developed a methodology for power plant synthesis, where the problem size is reduced using thermodynamic analysis. The problem size is primarily reduced in two ways; first by reducing the size of the superstructure and thus the integer variables and second by giving tighter bounds of the variables, and thus reducing the size of the search space. The methodology was applied to a chemical process plant by the author in the work by Tveit et al. [67]. Similar ideas were presented in the work by Hostrup et al. [32], where the focus was on chemical processes. A characteristic common to the methodologies mentioned above is that they all require a detailed mathematical model of all the units included in the superstructure.

Varbanov et al. [72, 73] used a combination of simulation and a successive mixed integer linear programming procedure, where values were fixed for the optimisation model and updated untill convergence after each run based on the results of more rigorous simulation. Iyer and Grossmann [33] developed a mixed-integer (MILP) formulation for the synthesis and operational planning of utility systems for multi-

period operation with varying demands that were solved using a bilevel decomposition algorithm. Francisco and Matos [25] claimed that by extending this bilevel decomposition algorithm to include global emissions of atmospheric pollutants, it is possible to obtain the best utility plant design using the equipment and fuel that not only minimises operational and capital costs, but also pollutant global emissions due to the combustion of fuels. Papalexandri et al. [50] integrated techniques for modelling and optimisation under conditions of uncertainty in order to explore flexible operating scenarios and energy management schemes of real industrial utility systems. Their method can be used both for small MILP and small MINLP problems. Chang and Hwang [13] developed a multiobjective MILP model for utility systems, where cost minimisation and global emissions where taken into account. Roosen et al. [53] used multiobjective optimisation for trading off investment and operating costs of a combined cycle power system.

Both genetic algorithms and evolution strategies have been used to optimise energy systems. For example, Valdés et al. [71] applied genetic algorithms to the problem of thermoeconomic optimisation of combined cycle gas turbine power plants, while Marechal and Kalitventzeff [44] applied genetic algorithms to the optimal integration of utility systems of chemical production sites. Lewin et al. [39] and Lewin [38] used a genetic algorithm for the synthesis of heat exchanger networks. In their work, both Roosen et al. [53] and Uhlenbruck and Lucas [69] used an evolution strategy for the optimisation of a combined cycle power plant. Toffolo and Lazzaretto [61] used an evolutionary algorithm for finding the optimal trade-off between energetic and economic efficiency of thermal systems.

Simulated annealing has been used the optimisation of energy systems. For example, Yu et al. [76] used a combination of genetic algorithms and simulated annealing for optimal energy integration of a large scale system. Painton and Diwekar [49] applied simulated annealing to find the optimal design of a gas turbine and Maia and Qassim [42] used simulated annealing to the problem of synthesis of utility

systems with variable demands.

2.3 Simulation of energy systems

Process simulation is a central part of computer-aided process design both in contemporary academic research and in industrial applications. A comprehensive review of simulators and simulation methods has been presented by Biegler [6] and Biegler et al. [8]. An extensive comparison between some current simulation programs relevant for the simulation of energy systems is presented in Giglmayr et al. [26].

Process simulator concepts have traditionally been classified into sequential modular methods and equation-oriented approaches. Sequential modular simulators are based on flowsheet topology of the black-box unit modules and on the calculation of the mass and energy balances for each unit. The units and the thermodynamic properties are often divided into sub-programs or processes. In a sequential modular simulator the program sets up the flowsheet topology of the units, inserts the input data and defines the calculation order of the unit modules in the process. Then the program calculates the mass and energy balances for each unit using the procedures defined in the unit operations library. Lastly, the physical properties of the streams, e.g. the steam properties such as entropy and enthalpy, are calculated using the physical properties library in the simulator. The major differences between the modular simulators are to be found in the libraries of unit operations and physical properties. Modular methods are widely used in process design work. The disadvantage of modular simulators is that they are inflexible for a large variety of user specifications in flowsheet design.

In the simulators based on the equation-oriented approach the unit equations are assembled and solved simultaneously using general solution strategies (e.g. Newton-Raphson or quasi-Newton methods). The program sets up the flowsheet of the

simulated process, organises the unit equations into one large set, and solves them with a general purpose equation solver. In the equation-oriented simulators there is almost no distinction between flowsheet or stream connection equations, unit operation equations and physical property equations. The advantages of equation-oriented simulators include being flexible in the flowsheet design and that they allow the use of advanced optimisation strategies. On the other hand, the performance of the equation-oriented methods is limited by the capabilities of the equation solver. Equation-oriented simulators also require large-scale numerical algorithms, good initial values and efficient strategies to prevent convergence failures. The main applications for the equation-oriented simulators are in the on-line modelling and optimisation fields.

Process simulation can be done either with a steady state or with a dynamic model. Steady state models are widely used in process design simulation. In addition, off-design simulations of the process in the loads differing from the design load are possible with steady state simulators. In order to also include the time dependence of the load variations in the simulations, a dynamic model is needed. Dynamic models are often used in on-line monitoring of the process, in planning of the optimal operation of the process and in diagnosis of operational faults in the process. However, if only design simulations or some off-design simulations without the time dependence of a process will be made, the performance of the steady state simulation programs is sufficient.

2.3.1 Simulation and optimisation

A common approach to improving processes using simulation is to simulate a number of cases, and then select the best of these. As this is often very time consuming and it is difficult to efficiently handle trade-offs, many commercial simulation packages have integrated NLP solvers for the optimisation of constrained continuous variables. For

example, both Aspen Plus by AspenTech Inc. and Balas by VTT Technical Research Centre of Finland use the *successive quadratic programming approach*[3] (SQP), which is an algorithm for solving NLP problems that is relatively easy to implement into sequential modular simulators. The SQP-methods use Newton's method to solve the Karush-Kuhn-Tucker optimality conditions for the NLP problem [2]. The resulting problem is a minimisation of a quadratic approximation of the Lagrange function where the constraints are linearised. For sequential modular simulation, many of the variables and equations can be hidden from the SQP solver using a black-box approach, thus reducing the problem size. For equation-oriented simulators the variables and equations are incorporated into the optimisation problem, resulting in a larger optimisation problem. Since the computation time for the SQP approach increases cubically with the problem size, it is rarely used in commercial equation-oriented simulators [8].

Solvers for MINLP problems have also been used in connection with commercial simulators. This is particularly useful in cases where the optimisation would need to include discrete events (*e.g.* if-then logical statements). An example of an MINLP solver used together with Aspen Plus is, for example, described in the work by Diwekar et al. [18].

The same computational and combinatorial problems mentioned in Section 2.2.1 apply to the algorithms for optimisation when they are implemented into simulators, and it is equally important to choose the correct algorithm for the optimisation. Equations that can be suitable for the simulators may have properties that are undesirable for optimisation algorithms. For these reasons it is often necessary to formulate the optimisation problem independently of the simulation model, in order to include equations with desirable properties and to be able to modify the optimisation model *ad hoc* to enable solvers to produce good solutions in a reasonable time.

[3]also known as sequential quadratic programming

2.4 Experimental design

The objective of *experimental design* is to develop a robust process for planning and conducting an experiment, analysing the results and obtaining objective conclusions. A good textbook on experimental design is that by Montgomery [46]. Experiments are often time-consuming and costly, thus a great deal of time has been spent developing methods to reduce the number of times different combinations of an experiment have to be performed. The focus in this work is on using experimental design strategies to develop a regression model (or models, in cases where one regression model is insufficient) based on a simulation model of an energy system.

In this respect an important methodology is the *response surface methodology*, which is an approach to process optimisation. This methodology starts with the development of a response surface, which is a functional relationship between the response and the independent variables. The response surface is then analysed, for instance, by the use of gradients. The process is sequential, so if necessary a new response surface is developed and analysed until the optimum operating conditions are determined. The response surface is in most cases a regression model, where the determination of the regression model parameters can be found using the proper experimental designs.

Possibly the most used designs are *factorial designs*, which are experimental strategies where factors are varied together, in contrast to one at a time. In the special case where k factors have only two levels (*i.e. 'high'* and *'low'*), the design is called a 2^k-factorial design [19]. The 2^k-factorial design can be used to generate linear regression models, and there are ready-made methods for estimating the regression coefficients according to the least-squares criterion. However, more data is needed in order to fit a quadratic model. A natural extension would be the 3^k-factorial design, where the k factors now have three levels (*i.e. 'high'*, *'intermediate'* and *'low'*).

However, the 3^k-factorial design is not the most efficient design for fitting quadratic models. There are many symmetric designs that could be used, for instance the *central composite design*, the *spherical composite design*, the *Box-Behnken design* or the *face-centred central composite design*. What the designs mentioned above have in common is that they can be used when the region of interest is cubical or spherical and the regression model is linear or quadratic. In cases where it is not possible to use these traditional symmetric designs, since the experimental region is irregular, the model is non-standard or the sample size requirements are unusual, other criteria for selecting the design must be applied. There are several design optimality criteria, of which perhaps the most used is the *D-optimality criterion*, and this is also being used in this work. A good introduction to D-optimal designs can be found in the paper by Aguiar et al. [16]. The symmetric designs mentioned above are all D-optimal designs.

The D-optimal design aims to minimise the volume of the hyper-ellipsoid that describes the confidence interval for each coefficient. When this volume becomes smaller, the coefficients become more precise, and subsequently also the estimation is more precise. For a given amount, n, of candidate points in the region of interest and a specific model to be fitted, the so-called *model matrix*, X, can be developed. The model matrix is a $(n \times p)$ matrix where p represents the number of coefficients in the model. The *dispersion matrix* is defined as $(X'X)^{-1}$, where X' is the transpose of the model matrix. The D-criterion states that the optimal design matrix, X^*, is the model matrix, X, that minimises the determinant of the dispersion matrix:

$$|(X^{*\prime}X^*)^{-1}| = \min_{X \in S} |(X'X)^{-1}| \tag{2.7}$$

where S is the set of all $\frac{n!}{p!(n-p)!}$ possible model matrices. The resulting design is subsequently D-Optimal.

Several exchange algorithms for finding D-optimal designs have been developed, of which perhaps *Fedorov's* algorithm is most known [22]. An overview of some

exchange algorithm can be found in the paper by Nguyen and Miller [47]. However, as the number of candidates increases the number of possible combinations become prohibitively large to be solved using the exchange algorithms and other strategies for solving the problem must be applied. Stochastic search methods based on natural processes like genetic algorithms and simulated annealing have successfully been applied to this problem. For instance Broudiscou et al. [10] used a genetic algorithm for selecting the D-optimal design, while Duffull et al. [20] used simulated annealing.

2.4.1 Simulation and experimental design

Experimental design has been used in connection with simulation modelling to a certain extent. The main focus seems to be on factorial designs and response surface methodology. In the book by Chung [15], a chapter is devoted to simulation and factorial experimental design. Spedding et al. [57] used a discrete event simulation model together with a factorial design and response surface methodology to determine the optimal configuration of a keyboard assembly cell. Dessouky and Bayer [17] used a combination of simulation and experimental design to minimise building maintenance costs. The simulation output was used in a factorial experimental design in order to identify the attributes that have the greatest impact on the costs. In the work by Kenne and Gharbi [34] simulation experiments were coupled with experimental design and response surface methodology to estimate the optimal control for a one-machine, two-product manufacturing system subject to random failures and repairs.

3 Objective and scientific significance

The objective of this work is to present a systematic procedure for analysing and designing energy systems. The procedure utilises simulation modelling, experimental design and regression models and mathematical programming. The procedure is able to simplify large problems so that they can be efficiently solved, but still preserve sufficient amount of details so that the objective of the analysis or design can be fulfilled. The main advantage of the methodology is that it can reduce the size of the problems in a way that is more flexible than existing methodologies using mathematical programming. The way the problem is reduced is not restricted by the thermodynamic aspects of the process, *e.g.* fixing steam pressures, or by requiring that all equations should be of a certain mathematical form, *e.g.* linear.

3.1 Earlier key developments compared to this work

Figure 3.1 shows an overview of the development stages of the concept compared to other strategies. The novel approach in the procedure is to systematically integrate a method for simplifying the problem by developing regression models based on simulations. As mentioned in Section 2.2.4, mathematical programming has been widely applied in the design of energy systems. Due to numerical or combinatorial problems, it is normally necessary to simplify the problems. Bruno et al. [11] simplified the optimisation models by fixing the pressures. By fixing the pressures the ability of the methodology to efficiently handle off-design situations of energy systems is reduced. The variation in pressure is for instance a very important part of steam turbine operation and design. Manninen and Zhu [43] and Hostrup et al. [32] reduced the optimisation model by thermodynamic analysis. By excluding solutions that are thermodynamically infeasible or obviously undesirable, it is possible to reduce the size of the problems by giving tighter bounds on the variables as well as

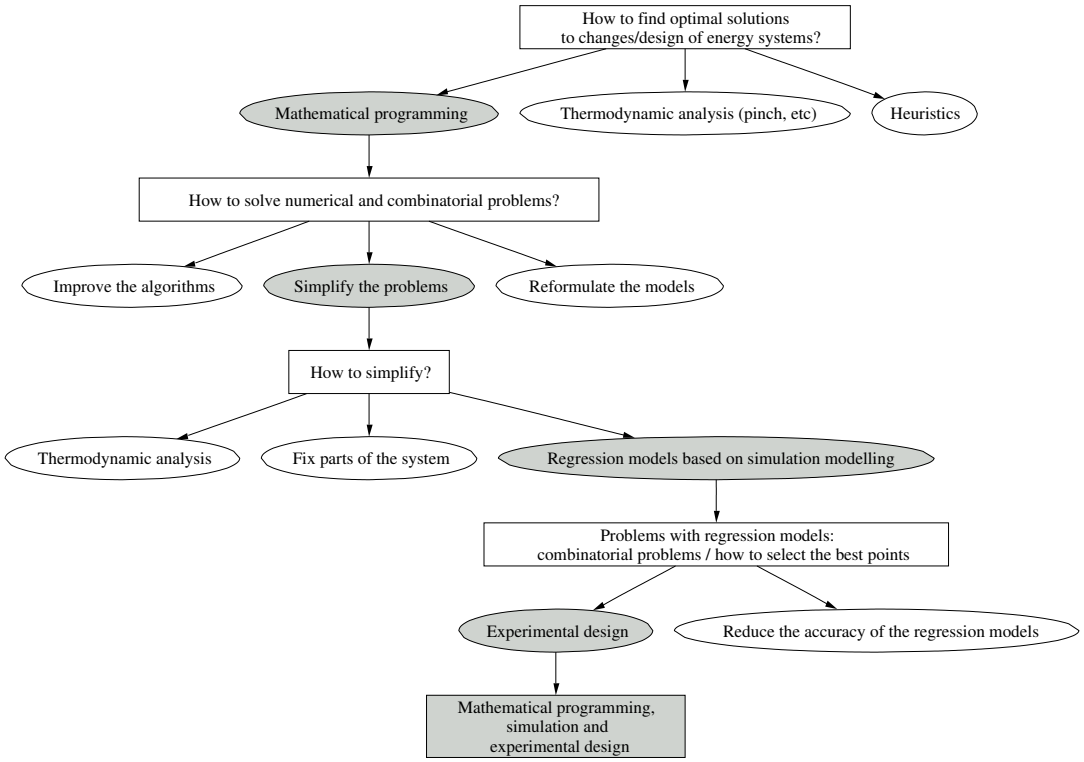

Figure 3.1: Overview of the stages of the development of the systematic procedure for the analysis and synthesis of energy systems.

reducing the size of the superstructures. However, all the units must still be modelled in detail, which can result in numerical problems if the equations are highly nonlinear and nonconvex. Iyer and Grossmann [33] simplified by modelling the system using only linear relations. By using only linear relations the nonlinearities in the system must be simplified or ignored, which might reduce the accuracy of the model.

The scientific significance of this work is that the problems mentioned above are avoided by using regression models based on simulation modelling together with experimental design to simplify the optimisation model. This enables greater freedom when simplifying the problems, without being bound by certain set of thermodynamic rules or the mathematical form of the problem, *e.g.* linear.

4 A systematic procedure for analysis and design of energy systems

The process of designing or analysing energy systems with the aim of achieving an optimal system involves many tasks and decisions. Many of these tasks and decisions are dependent on the methodology used, but more generic questions are independent of the methodology. In addition to the definition of the scope and objective of the design or analysis, some of the fundamental questions that must be answered are: *'What is the system and the system boundaries?'*, *'Which methodology or methodologies should be applied?'* and *'How can the models and results be efficiently verified?'* The quality and feasibility of the process, with respect to for instance time, is strongly dependent on these decisions. It is therefore important to have a good understanding of how the different steps and decisions affect the design or analysis process. The objective of this section is to give an overview of the procedure suggested in this work, with respect to the necessary tasks and decisions, and to summarise and connect the work in Publications I to VI. The development of the simulation model is primarily described in Publications I and II. The development of regression model for the systematic procedure is discussed in Publications II, IV, V and VI. Optimisation is discussed in all the Publications II to VI.

The systematic procedure presented in this work can roughly be divided into the following steps:

1. Development of the simulation model
2. Development of the regression model (including experimental design)
3. Development of the optimisation model

The purpose of the first step is to build a simulation model that is used to generate the data needed for the regression model(s). The next step will produce the regression model or models that are needed to get a representative optimisation model of the system. A simplified overview of the design procedure is presented in Figure 4.1.

The decisions made in all the steps also affect the previous steps as well as the

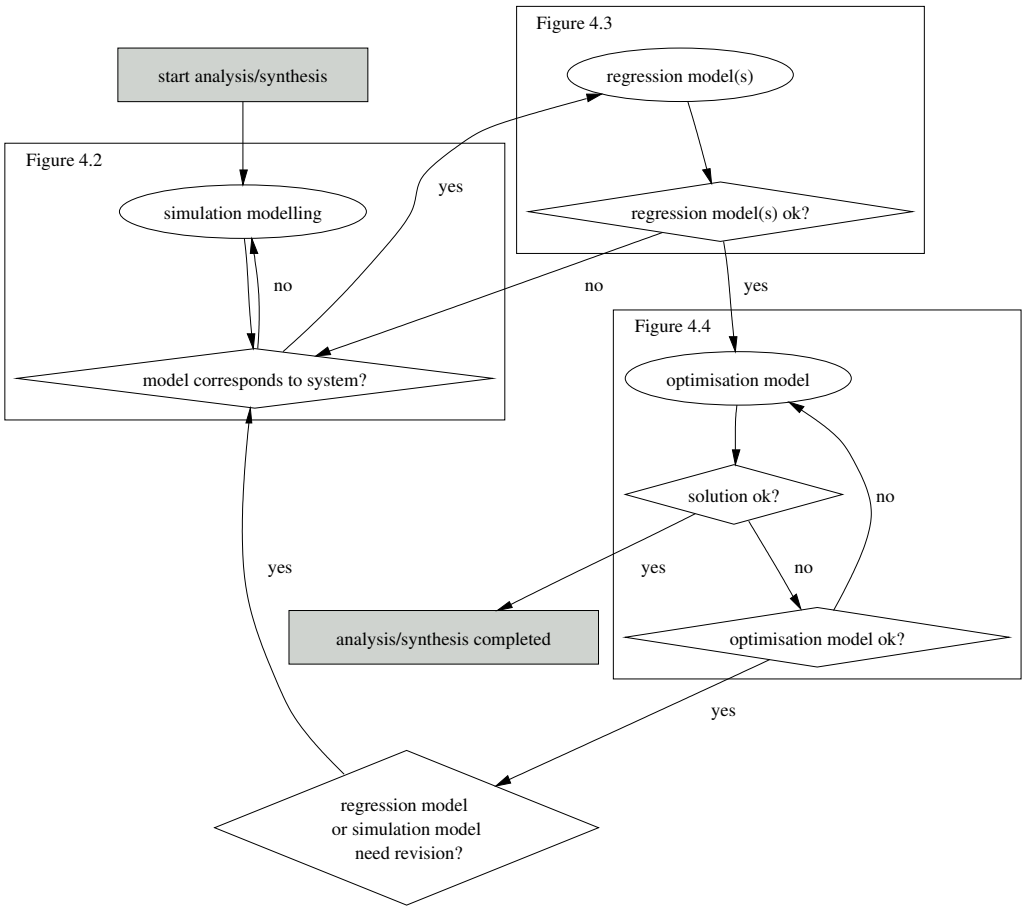

Figure 4.1: A simplified overview of the procedure for the analysis and design of energy systems. The different steps are shown in more detail in, respectively, Figures 4.2, 4.3 and 4.4.

next step. It is for instance quite possible that the information from the previous step contains faults or is insufficient. In these cases it is necessary to go back to the previous step or steps. The simplified steps of the procedure are presented in more detail in the following subsections. The simulation modelling is described in

Section 4.1, the development of the regression models are described in Section 4.2 and finally the development of the optimisation model is described in Section 4.3.

4.1 Simulation modelling

The development of a simulation model involves identification of the system being modelled, data extraction, the actual simulation modelling and the verification of the simulation model. An overview of the process is shown in Figure 4.2. The primary use of the simulation model for the systematic procedure presented here is to generate data for the regression model(s). For retrofit analysis, another natural source for data for regression models could be the monitoring system at the plant. However, there are many good reasons why data from a simulation model is preferable. For instance, in cases where the aim of the study is to evaluate structural changes to a system, the data from the monitoring system will only supply data from the existing system, which is of limited use. In Publication I the most important sources for data extraction for the simulation model of a sulphuric acid production process are listed and disussed. The use of simulation models and measurements at a plant as sources of data for the regression models is also discussed in Publication II. The data from the simulation model are based on the assumption that models of the different units are in energy and mass balance, which is rarely the case with data from monitoring systems. That the data is in mass and energy balance is important when considering both structural and parametric changes to a system. There are also many contributions to the unreliability of measured data; for instance, the measurements might be taken at different operation points, the instruments are not calibrated or are not working properly. Another source of error is that in many cases the measurements are not even meant to give absolute and accurate values, but rather to monitor changes in the process.

In addition to generating data, the simulation model can also be used for another

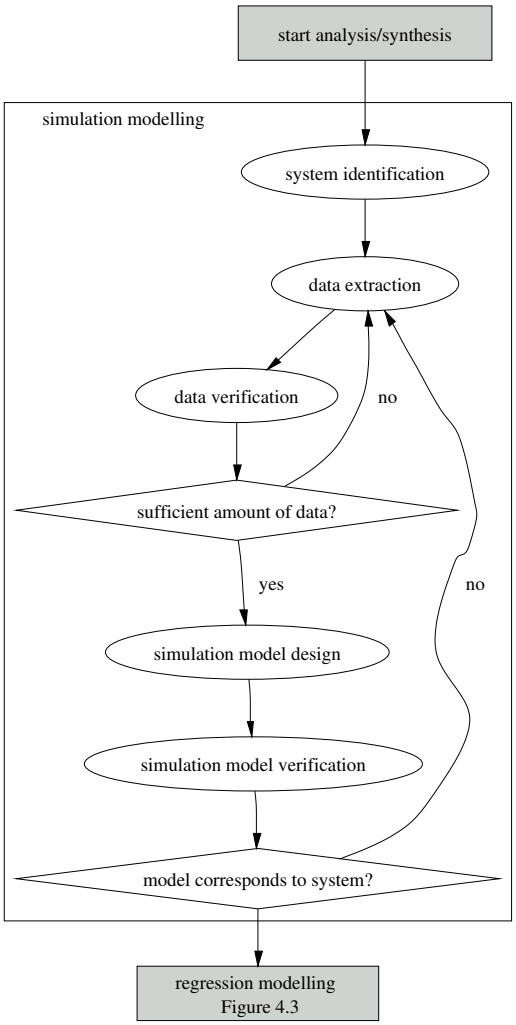

Figure 4.2: Overview of the process for the development of the simulation model.

purpose. Compared to an optimisation model, a simulation can be a better model of the system, which is due to the simplifications that are often necessary to make to the optimisation model. Another important use of the simulation model can therefore be to use the simulation model to verify the calculations by the optimisation model. This is discussed further in Section 4.3.

4.1.1 System identification, data extraction and data verification

In the context of simulation modelling, the system identification means to identify the boundary of the system, *i.e.* which are the units that belong to the system and what are the inputs and outputs of the system. At this stage it is also possible to estimate the level of detail for the simulation model, *e.g.* which part of the system can be left out of the analysis within the tolerances of the analysis. It is important to keep in mind during the development of the regression model that the target of the step is to make a realistic model of the system. This is discussed in Publication IV, where also a second order response surface model of the electrical efficiency of an indirectly fired microturbine is compared to a MINLP model where all the units are modelled in detail. With respect to the target of making a realistic model of the system there is a trade-off between a simple regression model that results in a more simple optimisation model and a more complex regression model that can give a more realistic model of the system, but also results in a more complex optimisation model.

When the system is identified, the next step is to extract data from the system. The data extraction is potentially the most time-consuming part of building a representative simulation model. There are two major problems with data extraction. The first problem is that all the necessary data might simply not be available. The second major problem is that in many cases the data that *is* available is ambiguous. It is important to notice that it is only possible to identify ambiguous data in the case where there is enough data to make an over-determined model. This is not always the case. As briefly discussed in the previous section, the ambiguity of the data can for instance arise when measurements are taken at different operation points, or when the measurements are incorrect. In many cases only the trends are valuable for the operation of the plant, so there is no need to get an absolute value from the measurements. This will be a problem when building a simulation model as it is in most cases crucial to get values that are in balance, or at least close to being in

balance. The above mentioned problems with the data extraction are difficult, if not impossible to avoid. This makes it also important and necessary to verify the data extracted.

It is a non-trivial task to verify the extracted data from a plant. For cases where time series are available, different statistical analysis can be applied to find the most probable set of values. In many cases the task is reduced to a matter of trust, *i.e.* which data seems unreasonable and which data can be trusted. The operating personnel of the plant usually have a good working knowledge of the process, so a good option would be to go through the data together with the operating personnel of the plant in order to identify possible ambiguities. This is the method used in the work presented in Publication I.

The verification of the data is normally an iterative process, since the validity of data can in most cases only be established when the simulation model is complete and the calculations can be compared to data extracted from the existing system. This is a part of the verification of the whole simulation model which is discussed in Section 4.1.3.

4.1.2 Simulation model design

For process simulators the simulation model design means to model the topology of the process and then to specify the behaviour of the units comprising the system. The way the topology and the behaviour of the units are implemented is dependent on the simulation software chosen. Although discussed in this section, the choice of simulation software is closely connected to the data extraction, as it determines what kind of data is needed. If the system being modelled is complicated, it might be difficult to identify all the data that is needed for the simulation model design beforehand, and it might be necessary to return to the data extraction step to obtain

enough data for the modelling. It is important to choose the simulation software that can model the system to the accuracy required, but at the same time the model of the system should be as simple as possible. If the simulation model is relatively simple, it means that numerical problems can be avoided. A simple model can also reduce the amount of data that is needed to be extracted and verified compared to a more complex model, and the verification of the complete simulation model will be easier. The verification of the simulation model is the next step to completing the simulation modelling.

4.1.3 Simulation model verification

The task of verifying a simulation model is very different if the objective is to model an existing system compared to if the objective is to model a new system (including major changes to an existing system). Both cases are discussed in this section.

For a simulation model of an existing system, verification can be made by comparing snapshots from the monitoring system at the plant with the similar values obtained from the simulation model. At this stage the data, on which the simulation model is based should also be verified. The problems with data from the monitoring system have already been discussed in Sections 4.1 and 4.1.1. An important problem is that it is next to impossible to obtain snapshots of the whole process from the plants to compare with the simulation model. This makes it considerably more difficult to verify how well the simulation model perform. However, it is possible to acquire a relatively good picture of how sensitive the simulation model is to changes in the parameters. One way to receive an indication of how the simulation model performs is to choose a few important values and compare these. A time series of these values would be necessary in order to be able to perform a valid statistical analysis, *e.g.* statistical and systematic error.

For a new system or for a system where the simulation model should model major changes, relevant data from a monitoring system is not available and other strategies for the verification must be applied. The verification could be achieved by analysing the simulation model, and then use engineering skills and heuristics to evaluate if the simulation model calculates the behaviour of the equipment as expected. This would require a good understanding of the system and the equipment. It is also possible to qualitatively compare data from a real similar system to the calculations by the simulation model.

Unless the simulation model is found to give a sufficiently good representation of the system, it will need to be revised.

4.2 Regression model for optimisation modelling

The process for the development of the regression model can be divided into two steps; first a decision about the form of the regression model must be made, second it should be decided how data for the regression model should be obtained and how the regression model should be fitted to the data. An overview of the process is shown in Figure 4.3.

The main decisions that have to be made when deciding the form of the regression model or models needed for the optimisation models are:

1. Decide which regression model or models that are needed
2. Decide which are the independent and which are the dependent variables
3. Decide the mathematical form of the regression model or models

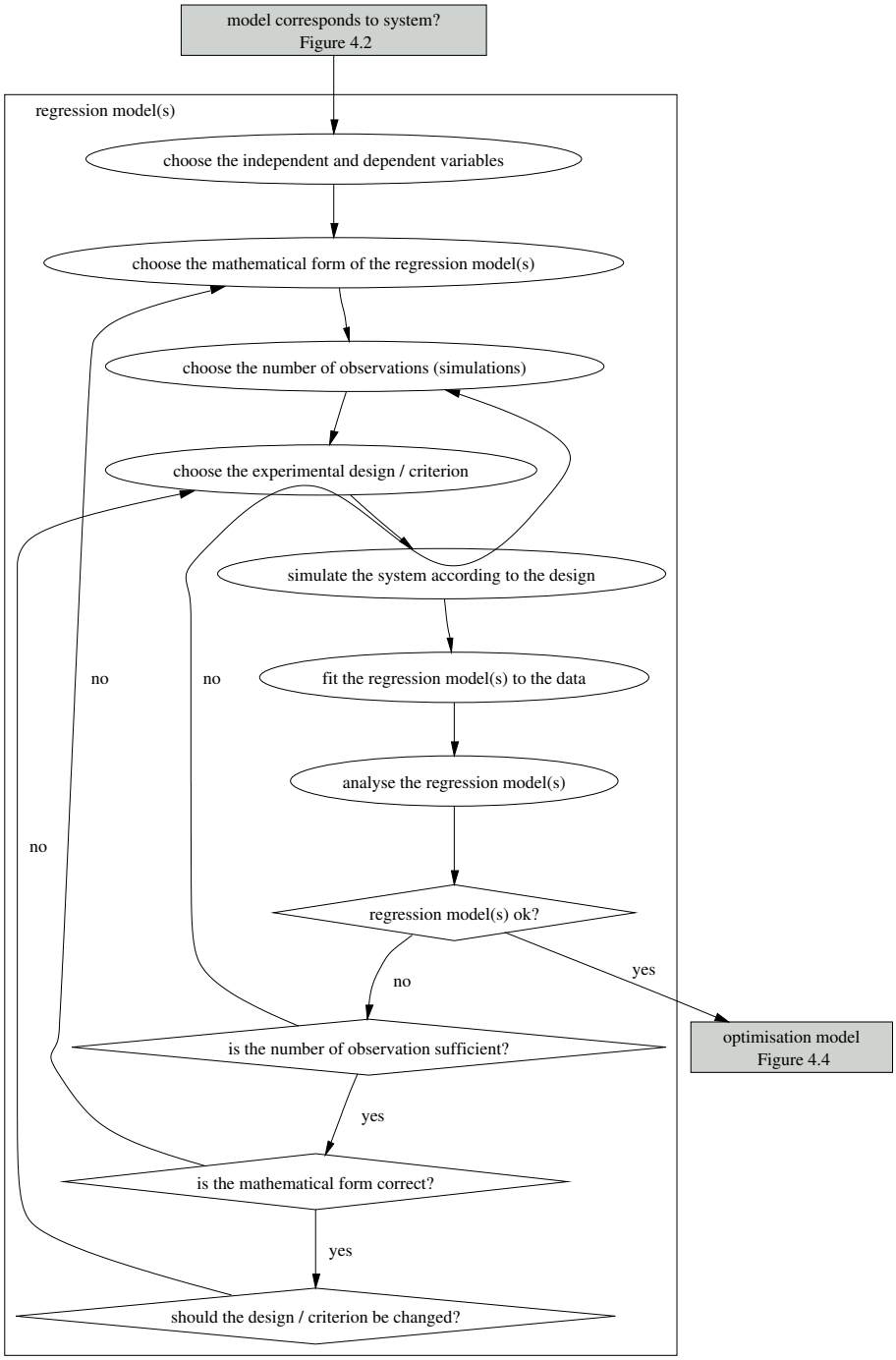

Figure 4.3: Overview of the process for developing the regression model.

These steps are closely connected to the design of the optimisation model, since the decisions must be based on the purpose of the optimisation model. When making these decisions it is important to keep in mind what the objective of the design or analysis is. The optimisation model must be designed to be a tool that can assist the achievement of the objective of the design or analysis of the energy system. If, for instance, the objective of an analysis is to maximise the electricity generated subjected to certain constraints, the regression model should be able to model a dependency between the generated electricity and the constraints. Consequently, the dependent and independent variables must reflect the dependency being modelled. The number of independent variables should be as small as possible, since the more independent variables the model has the more data is needed to fit the regression model.

In addition to the step where the regression model is fitted to the data, the mathematical form, *e.g.* linear, polynomial or logarithmic, of the regression model is needed when the decision about the way the data should be obtained is made. As a general rule the mathematical form of the regression model should be as simple as possible, and it should be able to model the dependency between the dependent and independent variables to a certain tolerance. For the optimisation model, it is in addition beneficial that the regression model is convex or easily convexified.

Discussions about some aspects of convex models related to the optimisation of energy systems can be found in other work by the author, namely in the work by Laukkanen and Tveit [37], Tveit [66] and Tveit et al. [68].

4.2.1 Data generation, fitting and verification of the regression model

A common approach to generate data from simulation models is to change one variable at the time and to keep the other variables of interest constant. This means

creating a grid of size n^k, where n is the resolution and k is the number of variables of interest. As the simulation model grows more complex, both the time to complete a simulation run and the number of variables will increase, and the combinatorial complexity increases exponentially. Due to the combinatorial complexity, the time it takes to complete a grid, makes it necessary to choose the values to be simulated more carefully. This can easily be appreciated even for relatively few variables. In the context of the systematic procedure presented in this work, the number of simulations, or observations, can be chosen in the following way:

1. Give an upper bound on the time that is reasonable to use for the simulation runs.

2. Calculate the number of simulation runs that are possible within this time, based on an estimate of the time it takes to complete one simulation run.

One option in order to select the values to be simulated is to take advantage of the methods developed in the field of experimental design, as described in Section 2.4. This is the option used in the systematic procedure described in this work. The objective of optimal experimental designs is to choose the best reduced set of points from all the possible candidate points. In Publications II, III and IV symmetric designs for fitting first order and second order models are applied as a part of the procedure for optimising energy systems. Publication II describes the development of a first order (bilinear) model using the 2^k factorial design, while Publication IV also describe the development of a second order response model using a face-centred composite design. In cases where it is not possible to use the traditional symmetric designs, since the experimental region is irregular, or the model is non-standard or the sample size requirements are unusual, other criteria for selecting the optimal design must be used. This is discussed in Publications V and VI, where the D-optimal criterion for selecting the design is applied.

When the best set of points to be simulated is chosen and the points have been simulated, the regression model must be fitted to the data. There are several ways of fitting the models, but two common criteria relevant to this work are the *least squares* (lsq) and *least absolute deviation* (lad) criteria. The objective of both criteria is to find the coefficients for the regression model that minimises the residuals. The criteria give rise to the optimisation problems shown respectively in Equations 4.1 (lsq) and 4.2 (lad).

$$\min\Big(\sum_{j=1}^{k} r_j^2\Big) \quad \text{s.t.} \quad y_j = f(\mathbf{x}_j) + r_j \quad \forall j \in (1, 2, \ldots, k) \tag{4.1}$$

where y and $\mathbf{x}$ are the dependent and independent variables respectively, $f(\mathbf{x})$ is the regression model being fitted to the data, r_j are the residuals, j refers to the data from the simulations and k is the number of observations.

$$\begin{aligned} &\min\Big(\sum_{j=1}^{k} r_j^+ + r_j^-\Big) \quad \text{s.t.} \\ &\qquad y_j = f(\mathbf{x}_j) + r_j^+ - r_j^- \quad \forall j \in (1, 2, \ldots, k), \quad r_j^+, r_j^- \geq 0 \end{aligned} \tag{4.2}$$

where r^+ and r^- are respectively the positive and negative residuals. In addition to the residuals, the variables in the optimisation problems are the coefficients of the regression model contained in $f(\mathbf{x})$. Due to the existing solvers, it is normally beneficial for the optimisation model to be convex. An additional constraint to Equations 4.1 and 4.2 could be that the eigenvalues of the Hessian matrix of $f(\mathbf{x})$ should be positive or equal to zero. A function with this property is positive semidefinite, and the addition of this constraint will consequently force the regression model to be convex.

The quality of the regression model must be tested after the previous steps have been performed. A natural way of testing the regression model is to compare a set of values of the regression model with values obtained from the simulation model. The set of values obtained from the simulation model should be different from the set of values used to fit the model. The values could be compared for the maximum

error (*i.e.* the maximum difference between the value calculated using the regression model and the value calculated using the simulation model), average error, standard deviation (*i.e.* indicate how the errors are distributed) and the square of the Pearson correlation. The square of the Pearson correlation indicates how well the values from the regression model explain the variance in the values from the simulation model. If the tests indicate that the regression model is not sufficiently accurate for the optimisation model, it needs to be revised. It might be necessary to improve the regression model by adding more data for the fitting or by changing the mathematical form of the model. It might also be necessary to add independent variables. If the regression model is found to be a good representation of the system, the next step is to develop an optimisation model.

4.3 Optimisation modelling

Optimisation modelling includes the formulation of the objective function and the constraints, the solving of the model using solvers that are suitable for the formulation and the verification of the solution found by the solvers. An overview of the process is shown in Figure 4.4. The formulation is strongly dependent on the objective of the analysis or design of the energy system. If, for instance, the objective of an analysis is to study how sensitive the economical feasibility of new investments are on the fuel and electricity spot-prices, the formulation will be different from a study where the objective is to reduce emissions of carbon dioxide. The objective and constraints of the optimisation model can be technical (physical) or economical. For a heat exchanger, the technical constraints can be the temperatures and the heat flow in the exchangers, while the economic constraints can be related to the installation and investment costs. Decisions about the formulation of the objective function and the constraints have already been made, as it is closely related to the development of the regression model or models in the previous step. As mentioned, simulation models are often better models of the system than optimisation models.

The advantage of using regression model based on simulations is that it is possible to reduce the size of the optimisation model compared to models where all units are modelled in detail, and it is also easier to develop an optimisation model that has certain properties, *e.g.* a convex model.

The choice of the optimisation algorithm or algorithms to solve the optimisation problem is an important part of the modelling. In order to obtain good solutions to the optimisation problem, the formulation of the model should be analysed and the choice of solvers should be based on this analysis. The choice of the optimisation algorithms (*i.e.* solvers) will in many ways also define the formulation of the optimisation model. In order to achieve an efficient model for the solvers, it is important to consider this, by analysing the model at all stages of the formulation. Again it is desirable to keep the model as simple as possible, as this will simplify the optimisation process. There is a trade-off between the need to keep the model as simple as possible and the need to get a realistic model of the system. As mentioned in Section 2.2.1, linear models are in most cases preferable to nonlinear, and convex models are preferable to nonconvex. When developing the regression model or models it is possible to choose mathematical forms that are suitable for optimisation. This is a distinct advantage of the models developed using the systematic procedure presented in this work compared to optimisation models where all the units are modelled in detail. A comparison between a model developed using the systematic procedure and a model where all the units are modelled in detail can be found in Publication IV.

In order to speed up the optimisation process, the simulation model can be used to find a good starting point for the optimisation. This is especially important for nonlinear models, and even more if the model is too large for the global solvers. For nonconvex models the starting point may determine the quality of the solutions. In some cases a good starting point might even determine if a feasible solution is even found. For complex optimisation problems it might be very difficult to find

a good starting point, or even a good feasible point. If the problem is kept small and simple, it might be possible to avoid the problems usually related to nonconvex models by using solvers that can guarantee global optimum. The solutions found by a global solver are not dependent on the starting point, but a good starting point will speed up the convergence time.

4.3.1 Optimisation model verification

The verification of the optimisation model and the results are an important part of the procedure, or indeed of any analysis or design of energy systems. The procedure presented in this work uses the assumption that it is possible to make a good simulation model of the system being designed or analysed. In previous sections it has already been discussed that it is normally possible for a simulation model to give a more accurate description of the system than an optimisation model. Assuming that this is the case, both the formulation of the optimisation model and the results can be compared to the calculations made by the simulation model. One way of verifying the formulations of the optimisation model is to fix the parameters of the optimisation model, solve the model and compare the results with similar calculations by the simulation model. If the calculations made by the optimisation model are similar within an accepted tolerance to the calculations made by the simulation model, it is a good indication that the optimisation model gives a good representation of the system. Otherwise the formulations must be revised, since it is possible that due to the simplifications, the solution found by the optimisation model is not feasible with respect to the simulation model and the actual system. This can be tested to a certain degree by feeding the result of the optimisation model to the simulation model and then comparing the results. Again a good correspondence between the calculations would indicate that the results are acceptable, and a poor correspondence would indicate that the formulations need to be revised. In addition to the simulation model, the verification of the results can and should be made by a

decision maker. For instance, the final verification of the results from the model can be made by letting engineers and operating personnel at the plant look at and comment the results. The decision maker can analyse the results based on the knowledge of the system, and decide if the calculations are reasonable and if the results are in correspondence with the objective of the analysis or design of the system. When the results of the optimisation model are found to be sufficient, the analysis or design of the energy system is complete.

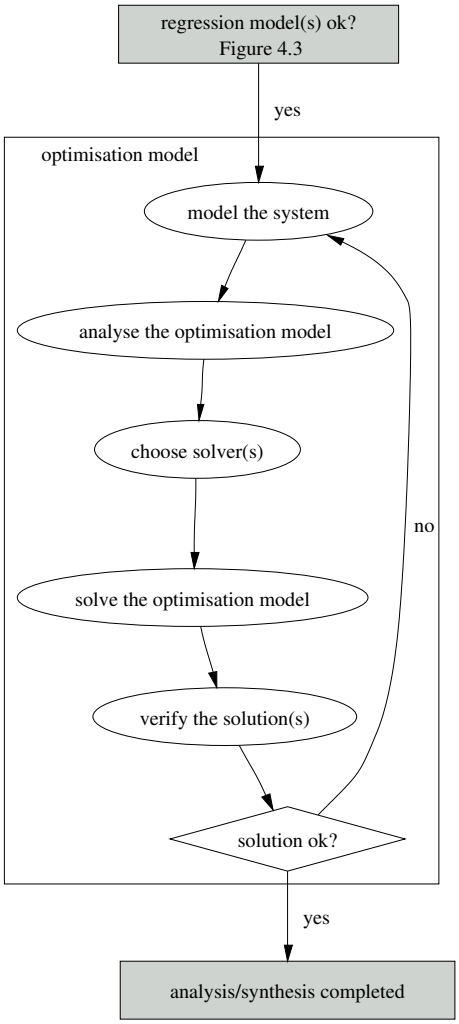

Figure 4.4: Overview of the optimisation modelling.

5 Conclusions

The objective of this work is to present a systematic procedure for analysing and designing energy systems. The procedure is presented in detail in Section 4 and in the Publications I to VI. The procedure utilises simulation modelling, experimental design, regression models and mathematical programming. Mathematical programming is used to find the best solutions in relations to the objectives of the analysis or design. The regression models based on simulation modelling are used together with experimental design to simplify the optimisation model, while at the same time maintaining a representative optimisation model of the system. The novel approach in the procedure is to systematically integrate a method for simplifying the optimisation problem by developing regression models based on simulations. The advantage of using a regression model based on simulations is that it is possible to reduce the size of the optimisation model compared to models where all units are modelled in detail, and it is also easier to develop an optimisation model that has certain properties, *e.g.* a convex model. The main advantage of the methodology is that it will present a novel option of reducing the size of the problems that is more flexible than the existing methodologies using mathematical programming. The way the problem is reduced is not restricted by the thermodynamic aspects of the process, *e.g.* reducing the size by fixing steam pressures, or by requiring that all equations should be of a certain mathematical form, *e.g.* linear.

5.1 Contribution of this work

The new requirements for cost efficient energy systems that have an efficient utilisation of energy with low negative environmental impact can only be met with efficient tools for analysing and designing energy systems. The systematic procedure can be used to quickly build a realistic optimisation model of an energy system to try to

achieve these goals. The procedure suggested in this work uses mathematical programming. The combinatorial and numerical problems associated with the use of mathematical programming for the analysis, design and synthesis of an energy system must be handled before any methodology can be efficiently utilised. In this procedure experimental design has been systematically used to guide the process points to be simulated. Experimental design has not previously been used in this specific context. The systematic procedure presented here addresses these problems of simplifying the optimisation problem by using regression models of the system. This is important, since it can efficiently reduce the complexity of the problem, and can thus be used to analyse and design complex energy systems with respect to several objectives. In this respect the procedure can be seen as a valuable addition to the existing methodologies.

The systematic procedure can be used for a wide range of problems for the analysis, design and synthesis of energy systems. For instance, the procedure can be used for the selection of the optimal pair of compressor and expander for a microturbine (Publication IV), for the investigation of integrating a pulp and paper mill with a municipal district heating network (Publication III) and for analysing the effect process changes will have on a complex utility system (Publications V and VI).

5.2 Recommendations and future work

The systematic procedure presented in this work is a good basis for further work and developments in the field of analysis and design of energy systems.

Important future work can be related to the evaluation of the accuracy of the models and the results, or to the data extraction. The evaluation of the models and results is an very important task of any modelling, and there is a need for efficient tools for evaluating the accuracy of the models and results. In addition to this, there is still

a great deal of work remaining to develop efficient tools for data extraction. Such tools would be valuable, as the data extraction can be a very time-consuming task when analysing and designing energy systems.

Further work could also involve developing the procedure presented in this work into a more formal framework. In addition to the steps introduced in this work, the framework should include a set of detailed rules for the procedure. The purpose of the set of rules would be to guide the analysis or design process in more detail.

References

[1] ARKI Consulting & Development A/S. SBB. Bagsvaerdvej 246 A, DK-2880 Bagsvaerd, Denmark. 26

[2] Bazaraa, M. S., Sherali, H. D., and Shetty, C. M. *Nonlinear Programming – Theory and Algorithms*, 2 ed. John Wiley & Sons, Inc, 1993. 24, 34

[3] Bejan, A. *Entropy Generation Minimization – The Method of Thermodynamic Optimization of Finite-Size Systems and Finite-Time Processes*. CRC Press, Inc, 1996. 23

[4] Bertsekas, D. *Nonlinear programming*, 2 ed. Athena Scientific, 1999. 25

[5] Beyer, H.-G., and Schwefel, H.-P. Evolution strategies; a comprehensive introduction. *Natural Computing 1*, 1 (2002), 3–52. 29

[6] Biegler, L. T. Chemical process simulation. *Chemical Engineering Progress 85*, 10 (1989), 50–61. 32

[7] Biegler, L. T., and Grossmann, I. E. Retrospective on optimization. *Computers and Chemical Engineering 28*, 8 (July 2004), 1169–1192. 30

[8] Biegler, L. T., Grossmann, I. E., and Westerberg, A. W. *Systematic Methods of Chemical Process Design*. Prentice Hall PTR, 1997. 32, 34

[9] Boyle, G., Everett, B., and Ramage, J. *Energy systems and sustainability – power for a sustainable future*. Oxford University Press, 2002. 17

[10] Broudiscou, A., Leardi, R., and Phan-Tan-Luu, R. Genetic algorithm as a tool for selection of D-optimal design. *Chemometrics and Intelligent Laboratory Systems 35* (1996), 105–116. 37

[11] Bruno, J. C., Fernandez, F., Castells, F., and Grossmann, I. E. A rigorous MINLP model for the optimal synthesis and operation of utility plants. *Institution of Chemical Engineers Trans IChemE 76* (1998), 246–258. 30, 38

[12] Center For Advanced Process Decision-Making, Department of Chemical Engineering. DICOPT. Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh, PA 15213, USA. 26

[13] Chang, C.-T., and Hwang, J.-R. A multiobjective programming approach to waste minimization in the utility systems of chemical processes. *Chemical Engineering Science 51*, 16 (August 1996), 3951–3965. 31

[14] Chou, C. C., and Shih, Y. S. A thermodynamic approach to the design and synthesis of plant utility systems. *Industrial and Engineering Chemistry Research 26*, 6 (1987), 1100–1108. 22

[15] Chung, C. A. *Simulation Modeling Handbook*. CRC Press, 2004, ch. 9 Experimental Design, pp. 9–1–9–12. 37

[16] de Aguiar, P. F., Bourguignon, B., Khots, M. S., Massart, D. L., and Phan-Than-Luu, R. D-optimal designs. *Chemometrics and Intelligent Laboratory Systems 30* (1995), 199–210. 36

[17] Dessouky, Y. M., and Bayer, A. A simulation and design of experiments modeling approach to minimize building maintenance costs. *Computers and Industrial Engineering, 43*, 3 (September 2002), 423–436. 37

[18] Diwekar, U. M., Grossmann, I. E., and Rubin, E. S. An MINLP process synthesizer for a sequential modular simulator. *Industrial and Engineering Chemistry Research 31*, 1 (January 1992), 313–322. 34

[19] Dougherty, E. R. *Probability and Statistics for the Engineering, Computing and Physical Sciences*. Prentice Hall International, Inc, 1990. 35

[20] Duffull, S. B., Retout, S., and Mentré, F. The use of simulated annealing for finding optimal population designs. *Computer Methods and Programs in Biomedicine 69* (2002), 25–35. 37

[21] El-Sayed, Y. M., and Evans, R. B. Thermoeconomics and the design of heat systems. *Trans. of ASME Journal of Engineering for Power 92*, 1 (January 1970), 27–35. 22

[22] Fedorov, V. V. Theory of optimal experiments. *Preprint No 7 LSM* (1969). lzd-vo Moscow State University, Moscow. 36

[23] Floudas, C. A. *Deterministic Global Optimization: Theory, Methods and Applications*, vol. 37 of *Nonconvex Optimization and its Applications*. Kluwer Academic Publishers, 1999. 26

[24] Floudas, C. A., Akrotirianakis, I. G., Caratzoulas, S., Meyer, C. A., and Kallrath, J. Global optimization in the 21st century: Advances and challenges. *Computers and Chemical Engineering 29* (2005), 1185–1202. 26

[25] Francisco, A. P. O., and Matos, H. A. Multiperiod synthesis and operational planning of utility systems with environmental concerns. *Computers and Chemical Engineering 28*, 5 (May 2004), 745–753. 31

[26] Giglmayr, I., Nixdorf, M., and Pogoreutz, M. Comparison of software for thermodynamic process calculations. *VGB PowerTech 2* (2001), 44–51. 32

[27] Grossmann, I. E., and Biegler, L. T. Part II. future perspective on optimization. *Computers and Chemical Engineering 28*, 8 (July 2004), 1193–1218. 30

[28] Haimes, Y. Y., Tarvainen, K., Shima, T., and Thadathil, J. On a bicriterion formulation of the problems of integrated system identification and

system optimization. *IEEE Transactions on Systems, Man and Cybernetics 1* (1971), 296–297. 28

[29] Hinrichs, R. A., and Kleinbach, M. *Energy – its use and the environment*, 3 ed. Brooks/Cole, 2002. 17

[30] Hohmann, E. C. *Optimum networks for heat exchange*. PhD thesis, University of Southern California, 1971. 23

[31] Holland, J. H. *Adaptation in Natural and Artificial Systems*. University of Michigan Press, Ann Arbor, 1975. 29

[32] Hostrup, M., Gani, R., Kravanja, Z., Sorsak, A., and Grossmann, I. E. Integration of thermodynamic insights and MINLP optimization for the synthesis, design and analysis of process flowsheets. *Computers and Chemical Engineering 25* (2001), 73–83. 30, 38

[33] Iyer, R. R., and Grossmann, I. Synthesis and operational planning of utility systems for multiperiod operation. *Computers and Chemical Engineering 22*, 7–8 (1998), 979–993. 30, 39

[34] Kenne, J. P., and Gharbi, A. A simulation optimization based control policy for failure prone one-machine, two-product manufacturing systems. *Computers and Industrial Engineering 46*, 2 (April 2004), 285–292. 37

[35] Kirkpatrick, S., Gelatt Jr., C. D., and Vecchi, M. P. Optimization by simulated annealing. *Science 220*, 4598 (May 1983), 671–680. 29

[36] Kotas, T. J. *The Exergy Method of Thermal Plant Analysis*. Krieger Publishing Company, 1985. 23

[37] Laukkanen, T., and Tveit, T.-M. Steam property functions suitable for mathematical programming. In *Proceedings of ECOS'03* (2003), N. Houbak, B. Elmegaard, B. Qvale, and M. J. Moran, Eds., vol. 3, Efficiency, Costs, Optimization, Simulation and Environmental Impact of Energy Systems, pp. 1735–1742. 49

[38] Lewin, D. R. A generalized method for HEN synthesis using stochastic optimization – II.: The synthesis of cost-optimal networks. *Computers and Chemical Engineering 22*, 10 (September 1998), 1387–1405. 31

[39] Lewin, D. R., Wang, H., and Shalev, O. A generalized method for HEN synthesis using stochastic optimization - I. general framework and MER optimal synthesis. *Computers and Chemical Engineering 22*, 10 (September 1998), 1503–1513. 31

[40] Lin, J. Multiple-objective problems: Pareto-optimal solutions by method of proper equality constraints. *IEEE Transactions on Automatic Control 21*, 5 (1976), 641–650. 28

[41] Linnhoff, B., Mason, D. R., and Wardle, I. Understanding heat exchanger networks. *Computers and Chemical Engineering 3*, 1–4 (1979), 295–302. 23

[42] Maia, L. O. A., and Qassim, R. Y. Synthesis of utility systems with variable demands using simulated annealing. *Computers and Chemical Engineering 21*, 9 (June 1997), 947–950. 31

[43] Manninen, J., and Zhu, X. X. Thermodynamic analysis and mathematical optimisation of power plants. *Computers and Chemical Engineering 22* (1998), S537–S544. 30, 38

[44] Marechal, F., and Kalitventzeff, B. Targeting the integration of multi-period utility systems for site scale process integration. *Applied Thermal Engineering 23*, 14 (October 2003), 1763–1784. 31

[45] Miettinen, K. M. *Nonlinear Multiobjective Optimization*. Kluwer Academic Publishers, 1999. 27, 28

[46] Montgomery, D. C. *Design and Analysis of Experiments*, fifth ed. John Wiley & Sons, Inc, 2001. 35

[47] Nguyen, N.-K., and Miller, A. J. A review of some exchange algorithms for constructing D-optimal designs. *Computational Statistics and Data Analysis 14* (1992), 489–498. 37

[48] Nishio, M., Itoh, J., Shiroko, K., and Umeda, T. A thermodynamic approach to steam power system design. *Industrial and Engineering Chemistry Process Design and Development 19*, 2 (1980), 306–312. 22

[49] Painton, L. A., and Diwekar, U. M. Synthesizing optimal design configurations for a brayton cycle power plant. *Computers and Chemical Engineering 18*, 5 (May 1994), 369–381. 31

[50] Papalexandri, K. P., Pistikopoulos, E. N., and Kalitventzeff, B. Modelling and optimization aspects in energy management and plant operation with variable energy demands-application to industrial problems. *Computers and Chemical Engineering 22*, 9 (1998), 1319–1333. 31

[51] Rant, Z. Exergie, ein neues wort fur technische arbeitsfahigkeit. *Forschung Ing. Wes. 22*, 1 (1956), 36–37. 23

[52] Reichardt, P. Ein neues Wärmeschaubild des Hochofens. *Archiv für das Eisenhüttenwesen*, 4 (August 1927), 77–101. 23

[53] Roosen, P., Uhlenbruck, S., and Lucas, K. Pareto optimization of a combined cycle power system as a decision support tool for trading off investment vs. operating costs. *International Journal of Thermal Sciences 42*, 6 (June 2003), 553–560. 31

[54] Ryoo, S., and Sahinidis, N. V. Global optimization of nonconvex NLPs and MINLPs with applications in process design. *Computers and Chemical Engineering 19*, 5 (May 1995), 551–566. 26

[55] Sierksma, G. *Linear and Integer Programming – Theory and Practice*. Marcel Dekker, Inc, 1996. 27

[56] Smith, E. M. B., and Pantelides, C. C. *Global Optimization in Engineering Design*, vol. 9 of *Nonconvex Optimization and its Applications*. Kluwer Academic Publishers, 1996, ch. -, pp. 355–386. Ed. Ignacio E. Grossmann. 26

[57] Spedding, T. A., De Souza, R., Lee, S. S. G., and Lee, W. L. Optimizing the configuration of a keyboard assembly cell. *International Journal of Production Research 36*, 8 (August 1998), 2131–2144. 37

[58] Statistics Finland. Energy statistics 2003, 2004. 17

[59] Szargut, J., Morris, D. R., and Steward, F. R. *Exergy analysis of thermal, chemical and metallurgical processes*. Springer Verlag, 1988. 23

[60] Tawarmalani, M., and Sahinidis, N. V. *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming*. Kluwer Academic Publishers, 2002. 26

[61] Toffolo, A., and Lazzaretto, A. Evolutionary algorithms for multi-objective energetic and economic optimization in thermal system design. *Energy 27* (2002), 549–567. 31

[62] Townsend, D. W., and Linnhoff, B. Heat and power networks in process design. part I: Criteria for placement of heat engines and heat pumps in process networks. *AIChE Journal 29*, 5 (September 1983), 742–748. 23

[63] Townsend, D. W., and Linnhoff, B. Heat and power networks in process design. part II: Design procedure for equipment selection and process matching. *AIChE Journal 29*, 5 (September 1983), 748–771. 23

[64] Tsatsaronis, G., and Moran, M. J. Exergy-aided cost minimization. *Energy Conversion and Management 38*, 15–17 (1997), 1535–1542. 23

[65] Tsatsaronis, G., and Park, M.-H. On avoidable and unavoidable exergy destructions and investment costs in thermal systems. *Energy Conversion and Management 43*, 9–12 (2002), 1259–1270. 23

[66] Tveit, T.-M. Steam turbine modelling for optimisation of CHP power plants. In *Proceedings of the 9th International Symposium on District Heating and Cooling 2004* (August 2004), T. Savola, Ed. 49

[67] Tveit, T.-M., Laukkanen, T., and Manninen, J. Application of a hybrid method for power plant optimisation. In *Proceedings of ECOS'01* (July 2001), A. Östürk and Y. A. Gögüş, Eds., vol. 2, Efficiency, Costs, Optimization, Simulation and Environmental Impact of Energy Systems, pp. 853–858. 30

[68] Tveit, T.-M., Savola, T., and Fogelholm, C.-J. Modelling of steam turbines for mixed integer nonlinear programming (MINLP) in design and off-design conditions of CHP plants. In *SIMS 2005, 46th Conference on Simulation Modeling* (October 2005), pp. 335–344. 49

[69] Uhlenbruck, S., and Lucas, K. Exergoeconomically–aided evolution strategy applied to a combined cycle power plant. *International Journal of Thermal Sciences 43*, 3 (March 2004), 289–296. 31

[70] GAMS, Ed. *GAMS – The Solver Manuals*. GAMS Development Corporation, 2004, ch. SBB. 27

[71] Valdés, M., Durán, M. D., and Rovira, A. Thermoeconomic optimization of combined cycle gas turbine power plants using genetic algorithms. *Applied Thermal Engineering 23*, 17 (December 2003), 2169–2182. 31

[72] Varbanov, P., Doyle, S., and Smith, R. Modelling and optimization of utility systems. *Chemical Engineering Research and Design 82*, A5 (May 2004), 561–578. 30

[73] Varbanov, P., Perry, S., Klemes, J., and Smith, R. Synthesis of industrial utility systems: cost-effective de-carbonisation. *Applied Thermal Engineering 25*, 7 (May 2005), 985–1001. 30

[74] Westerberg, A. W. A retrospective on design and process synthesis. *Computers and Chemical Engineering 28* (2004), 447–458. 19

[75] Whitley, D. An overview of evolutionary algorithms: practical issues and common pitfalls. *Information and Software Technology 43*, 15 (December 2001), 817–831. 29

[76] Yu, H., Fang, H., Yao, P., and Yuan, Y. A combined genetic algorithm / simulated annealing algorithm for large scale system energy integration. *Computers and Chemical Engineering 24*, 8 (September 2000), 2023–2035. 31

ISBN 951-22-8096-5
ISBN 951-22-8097-3 (PDF)
ISSN 1795-2239
ISSN 1795-4584 (PDF)