Synthesis and Optimisation of Large-Scale Utility Systems

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Declaration

The work described in this thesis is the original work of the author and was carried out without the assistance of others, except where explicit credit is given in the text. It has not been submitted, in whole or in part for any other degree at any university.
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Abstract

This research is focused on the simulation, optimisation and synthesis of utility systems, in particular combined heat and power (CHP) systems. These systems involve gas and steam turbines, steam generation at different pressure levels, condensing equipment and auxiliaries. The CHP systems are of substantial industrial interest for the efficient supply of heat and power. They are highly integrated and complex processes which are studied in an equation oriented (EO) framework including the models developed in this research.

An EO mathematical model for the simulation, optimisation and synthesis of CHP systems has been developed. It includes models for the simultaneous solution of all process streams, every major piece of equipment and investment and operating costs.

Several EO simulation examples, from simple unit operations, a whole real cogeneration plant involving a commercial gas turbine with 1450 variables and equations up to a synthesis model with 3,022 variables for a fixed structure, are used to demonstrate the applicability of the CHP model and the EO framework.

A number of energy and economic optimisation problems were solved using Sequential Quadratic Programming (SQP) methods. Both the EO model and the use of the more advanced SQP code (of the two used) were fully explored by experiments in a model with two steam turbines. In addition the following utility systems were optimised: a model of a combined heat and power plant; industrial size problems including a model for a cogeneration plant currently in operation and a synthesis model solved as continuous optimisation problem. The size of optimisation problems goes from about 100 to 3,042 modelling variables. The number of free variables goes from 4 to 98.

An important contribution made to solve EO simulation problems for CHP systems was to obtain converged solutions to plant sections which then were used as starting guess for larger plant sections until whole systems were simulated. Also this strategy was used to provide a warm starting guess for the efficient solution of large continuous optimisation problems of CHP systems.

Two synthesis problems were solved using a MINLP-BB (Mixed Integer Non-linear Programming with Branch and Bound) method. The problems of increased complexity consist of obtaining the optimum number and position of heat recovery (HR) exchangers that produce steam having the exhaust of a commercial gas turbine as the source of heat. The larger synthesis problem has 3,042 modelling variables, 98 of which were free variables. The problems consist of minimising the total cost of the system subject to a MINLP model.

The results obtained for the problems solved showed that the proposed EO model, the EO environment and the linked mathematical solvers represent a highly efficient approach to the simulation and optimisation of CHP systems. The synthesis problems' solution was not as robust as expected, but may be used for preliminary design stages of CHP systems.
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Chapter 1

Introduction

This chapter presents an overview of the characteristics and contributions of the research project together with some key definitions with which the project is concerned.

1.1 Background

Highly integrated processes (like utility systems) are characterised by a strong interaction between unit operations with multi-loop connectivities of material, energy and information. The design and optimal operation of these processes can be satisfied by a complex combination of alternatives. Such complexity represents an opportunity to apply modern mathematical formulations for their optimisation and synthesis.

Once the process model, the problem limitations and the criterion for improvement are defined in mathematical form this constitutes an optimisation problem. Some of the studies reported on the solution of large-scale continuous optimisation problems include an ethylene plant model with 8,500 variables (Rahabar et al., 1990) and mathematical test problems with up to 27,000 variables (Biegler et al., 1997b), (Lalee et al., 1998). Large-scale optimisation problems are best treated using sparse data structures for derivative information and include problems with a thousand or more variables (Lalee et al., 1998).

The optimisation problem when solved for practical applications in Process Systems Engineering is large-scale as the number of variables and equations describing the process model to an acceptable fidelity can be very large. The solution of a continuous optimisation problem for a
fixed process flowsheet structure provides the optimum value of the objective function as well as of the free variables and the value of all the modelling variables which satisfy the modelling constraints and limitations.

As stated in (Biegler, 1992), the general optimisation problem may contain continuous and integer variables as well as nonlinear algebraic equations, thus it is termed a mixed integer non-linear programming (MINLP) problem. In synthesis problems the optimal structure and number of equipment items within a process as well as the continuous variable optimisation are found. The solution of a synthesis problem provides the designation of the structure of the system elements that will meet the designers’ goals.

An important area in synthesis and optimisation is the problem of utility systems. A utility system consists typically of several unit operations, such as fired or waste heat steam generators, steam turbines, condensers, pumps, compressors, gas turbines, etc. These systems can be represented by a flowsheet and can supply electric and mechanical power, heating and cooling demands. This research has special relevance to combined heat and power (CHP) systems in particular combined cycle and cogeneration plants.

Problems in design and optimisation of industrial utility systems have been addressed using methods which include: heuristics for the design of steam generation and distribution systems (Peterson and Mann, 1985); a design qualitative procedure for the use of heat engines and heat pumps, based on heuristics and thermodynamic approaches (Townsend and Linnhoff, 1981); mixed integer linear programming (MILP) (Papoulias and Grossmann, 1983a); the use of linear programming (LP) coupled with dynamic programming (Petroulas and Reklaitis, 1984) for the synthesis and design problem of plant utility systems; the use of non-linear programming (NLP) employing sequential linear programming (SLP) for the optimisation problem, and MILP for the operational strategy of a combined cycle plant (Yokoyama et al., 1994); modular simulation for single or combined cycle power plants (Falcetta and Sciubba, 1995); simulated annealing for the synthesis of utility systems (Maia et al., 1995) and a MINLP model for synthesis and operation of these systems considering fixed heat and power demands and selected pressure levels (Bruno et al., 1998). There is however, no reported specialised application of the equation oriented (EO) approach 1 to modelling, simulation, optimisation and synthesis of CHP systems leading to large-scale problems. In particular, there are no approaches involving an extensive set of fundamental rigorous and realistic models with many useful variables for all relevant process streams and unit operations as well as investment and operating costs. Models are required

---

1 details of the EO approach are given in Section 1.1.2.
whose equations can be solved simultaneously for problems in CHP systems up to industrial size dimensions. And that is what is this thesis about.

The other highlight of the investigation presented here is that many of the papers on the EO approach, from early work in EO flowsheeting (Westerberg and Berna, 1978) to more recent research e.g. (Mallya et al., 1997) in EO simulation and optimisation, mainly consider flowsheets involving distillation columns. In this thesis we show the application of the EO approach to a number of CHP systems including a real cogeneration plant currently in operation (Gator-Power, 1994).

Although synthesis and optimisation are the main areas of this research, we solved large-scale simulation problems too. This was in order to test the applicability of the proposed models, to demonstrate the usefulness of our new EO modelling environment and to provide warm-starting guesses for the efficient solution of NLP optimisation and synthesis problems.

1.1.1 Combined heat and power (CHP) systems

There remains considerable interest in solving utility systems design and optimisation problems, in particular CHP systems where electricity and process heat and/or mechanical power are produced from the same primary energy source. The industrial energy sector worldwide has considerable interest in expanding the application of CHP systems due to their environmental and economic advantages and their high reliability compared with other energy producing systems (Najjar and Akyurt, 1994).

In the more complex CHP systems considered in this study a gas turbine (GT) is used to produce electric power and its exhaust is used in a heat recovery steam generator (HRSG) that produces steam at different pressure levels. The steam can be used in steam turbines for producing additional electricity or mechanical power and/or for the supply of heat loads in a process plant. In the CHP plants of this research a system with both gas and steam turbines is called a 'combined cycle' while a system without steam turbines is termed a 'cogeneration plant'.
1.1.2 Sequential modular vs. equation oriented (EO) approach

In order to introduce the sort of strategy followed to solve the simulation, optimisation and synthesis problems of utility systems, it is necessary to provide a brief review of simulation strategies. Steady state simulation programs are used for process design, see e.g. (Bogle and Pantelides, 1988). These programs are known as flowsheeting programs for which there are two approaches:

- **Sequential modular approach.** The subroutines for each unit operation are solved sequentially. Each unit operation is represented by a subroutine that calculates outputs, given inputs and parameters. The units are calculated in the order given by the flow diagram. The process is represented by a collection of modules (a module is a model of an individual element in a flowsheet) in which the equations representing each subsystem are collected together and their solution coded so that the module may be used in isolation from the rest of the flowsheet.

- **Equation oriented (EO) approach.** Models for process streams, unit operations, and a criterion for improvement (in the case of optimisation problems) constitute the system model. The problem is set up as a set of independent simultaneous equations to be solved. All modelling equations are assembled as a large set of nonlinear algebraic equations. An occurrence matrix that represents the model of a utility system is a sparse matrix (see the schematic representation in Fig. 1.1), where individual equations, e.g. a pumping power calculation, contains a small subset from the whole modelling variables. In simulation problems the number of variables equals the number of equations. Thus such a matrix is square. A great advantage of the equation oriented approach is that any variable may be set or calculated whether it is an input, output or parameter. This gives a considerable advantage over the sequential modular approach. In EO optimisation there are free variables and the entire set of equations (and inequalities) representing the process is employed so that the process model equations form the constraints for the optimisation of a suitable objective function.

In the EO optimisation and synthesis approach the optimum variables of the system are found while simultaneously moving toward the solution of the set of algebraic equations that model the system.

The EO approach allows flexibility in process specifications, and tends to be an effective way of solving highly integrated flowsheets where the unit operations interact strongly.
1.1.3 In-house computer programs for the EO approach

The early stages of this research included the use of tailor-made Fortran 90 programs to create the utility system optimisation model, which was solved with a particular sequential quadratic programming (SQP) solver described in Chapter 4, Section 4.2.1 (Zoppke-Donaldson, 1995). However as the size and complexity of the problems solved increased this motivated the use of a modelling system (Mitchell and Morton, 1996) named the Flexible Modelling System (FMS), described in Chapter 5, Section 5.1. FMS provides an EO modelling environment for general Process Systems Engineering problems, and can be linked to a variety of analysis tools and solvers as detailed below. With FMS, complex unit and network models can be built from a set of unit operation and stream models. Starting guesses are easily given for problems of any size, including 'warm starts' which are solutions or partial solutions of sub-models.

A number of tools have been linked to FMS and used in the work reported here. They include:

1. an Equation Analyser (EA) described in Chapter 4, Section 4.1.1, that checks for modelling errors leading to redundant equations and allows the identification of free variables in a given model (Morton and Collingwood, 1998);

2. a new sparse Nonlinear Algebraic Equations (NLAE) solver which aims to
provide increased robustness over Newton's method by the provision of a singular equation solver, reordering strategies and a trust region (TR) to control step size (Morton, 1997). More details are given in Chapter 4, Section 4.1.2;

3. the filterSQP solver is an advanced nonlinear programming optimisation package from Prof. R. Fletcher's group at Dundee University in Scotland. It is a SQP trust region algorithm with a 'filter' strategy aimed to promote global convergence (i.e. from any starting point). The 'filter' is a list of pairs of objective function values and norms of constraints violations (Fletcher and Leyffer, 1998). See Chapter 4, Section 4.2.2 for more details.

4. a MINLP_BB solver that is a mixed integer non-linear programming solver with a branch and bound strategy for the integer variables and the filterSQP method for the NLP subproblems optimisation (Leyffer, 1998). Chapter 4, Section 4.3 provides additional details.

1.2 Problems description

As seen in the literature search (Chapter 2) the simulation, synthesis and optimisation problems in utility systems have been solved in separate cases, using different methodologies. These include heuristics, modular simulation, targeting approaches and mathematical formulations involving linear and nonlinear models, but generally few modelling variables. There is then scope for the application of an EO environment linked to powerful optimisation and synthesis codes, which in turn needs fundamental EO models with many variables and nonlinearities, for the sake of better modelling. As mentioned, having these EO models requires us to solve EO simulation problems in order to test models and provide suitable starting guesses for the optimisation and synthesis problems.

The widespread use in industrial practice of recent efficient mathematical codes for the solution of large-scale optimisation and design problems in utility systems is not known, as reported in the literature survey. These kind of codes are focused on equation oriented approaches to optimisation and synthesis whose use is limited in industry.

Thus the problems concerned in this research refer to the simulation, optimisation and synthesis of utility systems in an EO approach. We tested a proposed model for these systems as well as the efficiency of a new modelling system and of the new mathematical codes linked to the
modelling system. A brief explanation of the sort of problems solved is:

○ **Simulation problems.**
  
  In EO simulation a large sparse set of nonlinear algebraic equations is solved. The model of a whole CHP plant constitutes a non-trivial system of equations to be solved and requires a reliable Newton-type solver. For a successful solution of a simulation problem there should be no redundant equations nor free variables. The efficiency of the solver as well as a strategy for providing a starting guess also play an important role.

○ **Optimisation problems**
  
  The optimisation of utility systems involves an objective function for minimising energy consumption or total costs subject to constraints given by the system model. This is given by a large set of nonlinear and some linear equations and by bounds on variables.

  In this research, for a given utility system we have a nonlinear objective function (O. F.) and the plant contains nonlinear equations. Thus, the problem must be formulated as a nonlinear programming (NLP) optimisation problem.

  The objective function is optimised simultaneously with the satisfaction of the constraints as the continuous free variables reach their optimum values.

  The generation of a suitable starting guess for successful convergence of CHP optimisation problems is also an issue which needs to be addressed.

○ **Synthesis problems**
  
  This problem consists in finding an optimal process flowsheet by solving a synthesis model having continuous and integer variables.

  The synthesis model is a MINLP problem that involves the representation of alternatives in a hyperstructure (Floudas, 1995) where all process alternative structures are considered.

1.3 **Research objectives**

The interest in this research is focused on utility systems simulation, optimisation and synthesis in an EO approach. The particular objectives can be enumerated as follows:

○ Develop mathematical models involving twice-continuously differentiable equations for their simultaneous solution for a considerable number of unit operations, for process
streams, for energy efficiency, and for investment and operating costs in utility systems. In particular we focus on combined heat and power systems because of their level of industrial interest and economic advantages. For such models consider rigorous as well as mathematical descriptions which are realistic (using current design practice). The system model should consider the steady state and be represented by a large set of nonlinear algebraic equations.

- In order to use these models for simulation, optimisation and synthesis by an EO approach obtain the exact 1st and 2nd partial derivative information to be supplied to the different mathematical codes to be used.

- Propose models for EO simulation from single unit operations up to industrial scale utility systems. Evaluate their usefulness as well as the efficiency of the in-house process modelling language, named the Flexible Modelling System (FMS) (Mitchell and Morton, 1996), to construct the plant models. In the process of solving the EO simulation problems test the applicability of the Equation Analyser (EA) (Morton and Collingwood, 1998) that checks for the existence of redundant equations and free variables. In addition demonstrate the efficiency and robustness of the new sparse Nonlinear Algebraic Equation (NLAE) solver (Morton, 1997) interfaced to FMS for solving large problems.

- Find an appropriate strategy for solving large utility system’s simulation problems by simultaneous equations.

- Since FMS did not have the required interconnection with all the desired mathematical codes for this research (namely for optimisation and synthesis), complement the existing filterSQP/FMS interface for NLP optimisation and then interface the MINLP.BB solver to FMS for solving synthesis models.

- Propose models for the EO continuous optimisation of utility systems. In an early stage use a tailor-made set of Fortran 90 programs to create the plant model. To initially test the proposed EO optimisation models use the SQP solver with a ‘tolerance-tube’ approach described in (Zoppke-Donaldson, 1995). As the research progressed we used FMS for modelling and the filterSQP code (Fletcher and Leyffer, 1998) for solving optimisation problems.

- For the optimisation problems use different criteria for improvement, such as efficient use of energy and economic optimisation.

- Find a suitable strategy for initialisation of large-scale optimisation problems.
Demonstrate applicability of the proposed models for the NLP optimisation of CHP systems up to industrial scale size. Likewise demonstrate the efficiency of the new filterSQP solver and the usefulness of the Flexible Modelling System (FMS) for modelling complex optimisation problems.

For the synthesis problems propose a suitable MINLP model for utility systems. Include the process model, integer and continuous variables and logical constraints.

Test the proposed MINLP model as well as the efficiency of the MINLP_BB solver (Leyffer, 1998) for large CHP systems models.

Evaluate the convenience of using detailed against approximate models in large synthesis problems in utility systems.

1.4 Solution strategy

Since CHP systems are described by highly integrated processes we decided to study them in an equation oriented (EO) approach for solving simulation, optimisation and synthesis problems.

Our EO environment includes FMS and a set of suitable mathematical solvers. The use of the EO environment presents the advantage that the variables are bounded so that the solution of the equations can be prevented from diverging excessively at any point. This is very important since different equations from the process model are only valid for a range of values physically and/or mathematically reasonable.

Utility systems problems are represented by a sparse nonlinear system of equations. Thus it was necessary to use sparse versions of the solvers in the EO approach to reduce the storage space for matrix manipulation and to save computation time (compared to the use of solvers in dense version \(^2\)).

A Newton-type method was used for solving the problems in this research and exact analytical derivatives where obtained using Maple V, a commercial programme for symbolic algebraic and numerical manipulation.

The general strategy followed for models creation, solution of simulation, optimisation and synthesis problems is given in the following sections.

\(^2\) where all elements of the model matrix (including zeros) are stored and manipulated.
1.4.1 Creation of models

In EO models of heat and power systems, the equations represent the balances and performance models for unit operations, and also relationships between variables in process streams (if more than a minimal independent set is used). Equipment and process streams models are represented by a set of independent non-linear algebraic equations. Mathematical models for simultaneous solution for the many process streams, unit operations and criteria for improvement (i.e. objective functions) were proposed, implemented and tested. A full explanation of how these models were created and the actual models are presented in Chapter 3 and in Appendices A - D.

The process model developed consist of:

- **Streams definition**, including connecting variables between unit operations. The stream models use a set of thermodynamic subroutines involving twice-continuously differentiable equations for the physical properties relevant in heat and power systems. First and second derivatives of these quantities are returned by the physical property subroutines for use with the mathematical solvers. Our rigorous water/steam stream definition (described in Chapter 3 Section 3.1.1. and Appendix A) contains 9 equations and the following 12 variables: \( F, P, h, H, T, s, \phi, q, T_s, h_f, h_g, v \), namely mass flow, pressure, specific enthalpy, enthalpy flow, temperature, specific entropy, vapour fraction, stream quality, saturation temperature, enthalpy of saturated liquid, enthalpy of saturated vapour and specific volume. A smoothed equation relating \( \phi \) and \( q \) was included for being able to describe a stream using the same definition in liquid, vapour or in the two phase region.

For further details of this and the other proposed stream models, see Chapter 3, Section 3.1 and Appendices A - C.

- **Unit operation models.** Every model has:
  - Material Balances.
  - Energy Balances.
  - Momentum Balances or pressure relationships.
  - Performance equations.

- A relevant energy or economic minimisation **objective function** for optimisation and synthesis problems.
The extension of a previously presented model for utility systems (Morton, 1994a) was developed in this research to consider CHP systems. Some of the initial results are in reported in (Morton and Rodríguez-Toral, 1997), (Rodríguez-Toral et al., 1999a) and (Rodríguez-Toral et al., 1999b).

1.4.2 Simulation

The models for each problem were constructed in FMS, using equation based models as described in the last section.

In an EO approach process models invariably contain more variables than equations. The difference equals the number of degrees of freedom and in order to simulate a system a specification, or fixed variable value, must be given for each degree of freedom in the initial model.

Each model was run through the EA to check the formulation and identify a possible set of specified variables. All simulations were performed with the sparse NLAE solver mentioned above.

In the initial solution stage of a given simulation problem a default initial guess was defined in FMS for each type of variable and used to start the solution. For more complex simulations the default values did not allow the problem to be solved, thus "warm-start" initial guesses were used by overwriting the default guesses with converged values from separately solved subsystems. Details are included in Chapter 6.

1.4.3 Optimisation

In EO optimisation there is great flexibility to choose different sets of fixed variables, and consequently the free variables or design variables. This makes the EO approach an attractive way to solve engineering problems. In contrast, the sequential modular approach has been a popular way to analyse heat and power systems with industrial size gas turbines (Falcetta and Sciubba, 1995), (Seyedan et al., 1995), (Ong'iro et al., 1996). There tends to be a computational penalty in selecting specifications which can cause information flow to take place against the material flow of the system.

For solving the continuous optimisation problems we selected a NLP method which is a SQP
method. SQP methods are suitable for large-scale problems (Biegler, 1992).

In modelling utility systems, the second derivative matrix in the Quadratic Programming (QP) problem becomes very large. When update formulas, such as positive definite BFGS, \(^3\) are used to approximate the second derivative matrix, a very large and dense matrix has to be stored and updated at every iteration. To avoid this problem exact second derivatives and NLP sparse solvers (which use only non-zero elements) were employed.

The large number of variables and modelling equations involved in EO optimisation requires a sparse matrix representation of the problem. This in turn requires the use of special mathematical techniques for continuous variable optimisation. The high degree of nonlinearity of many of the modelling equations as well as the existence of non-smooth functions also imposes special demands upon the solver. For large-scale problems, the solver should be able to handle sparse matrix representations of the first and second partial derivatives (Jacobian and Hessian matrices respectively) which are needed in the NLP solution method.

In order to solve successfully large NLP optimisation problems a warm starting guess obtained by simulation was supplied to the filterSQP optimiser.

1.4.4 Synthesis

Based on fundamental rules for superstructure creation, a flowsheet is specified and a solution containing optimal structure and continuous variable optimisation was obtained by solving the MINLP model proposed in this research. The MINLP model contains the relevant plant model used for the NLP optimisation problems, integer variables for the heat recovery (HR) exchangers in a HRSG and logical constraints.

The MINLP solver has a branch and bound strategy for the integer part of the model and uses the filterSQP for NLP subproblems.

1.5 Research scope

In the simulation, synthesis and optimisation tool for utility systems developed, any variable of the system (temperature of high pressure superheated steam, imported utilities, power generated...)

\(^3\) (Broyden-Fletcher-Goldfarb-Shanno), see e.g. (Biegler, 1992).
ation, capital or operating costs, etc.) may be optimised. This is a great advantage compared with simulation by the traditional modular approach (presumably most used for the commercial design of utility systems), where only the input variables to the models are used for the simulation and there is less flexibility to perform calculations in many ways as in NLP optimisation.

An extensive set of example problems solved for EO simulation, NLP optimisation and MINLP synthesis are presented in this thesis.

Some of the equations in the water/steam model are non-smooth. A special smoothing procedure was used to approximate these with smooth polynomials which the NLP can handle.

Simulation problems presented in Chapter 6 include single streams and unit operations; a real cogeneration plant (Gator-Power, 1994) and a large synthesis model for a fixed structure with 3,022 variables and equations. The use of an Equation Analyser (Morton and Collingwood, 1998) for checking that an EO model is well defined, and the use of a new sparse NLAE solver (Morton, 1997) proved to be very effective for the solution of the utility systems simulation models. The difficulty of converging a large sparse system of nonlinear equations (e.g. for an industrial plant model) was overcome by adopting a strategy in which partial solutions were obtained for sub-sections of the plant.

Optimisation was studied by solving NLP problems where thermal efficiency or cost minimisation was the relevant objective function, problem sizes range from about 100 up to more than 3,000 variables. The several optimisation examples which were built from EO models for each unit operation include a model of a combined heat and power plant that has a steam system and a process air supply system. For this example the NLP optimisation code used is shown to work efficiently. This code uses a recent implementation of the Sequential Quadratic Programming (SQP) method (Zoppke-Donaldson, 1995), which uses a 'tolerance tube' to decide whether or not each step solved by a QP point approximation of the NLP is acceptable. Further to the development of this SQP method an advanced SQP solver named filterSQP aimed at promoting global convergence (Fletcher and Leyffer, 1998) from Roger Fletcher's group at Dundee was available to our research group. Thus it was interfaced to FMS (Mitchell and Morton, 1996) and several NLP optimisation examples were solved including:

- problems on the effect of the initial trust region size
- problems on the effect of scaling variables, constraints and derivatives upon the solver performance
the use of dense and sparse filterSQP versions was compared; and

an analysis of the 'shadow price' of the high pressure (HP) steam temperature was performed

All of these problems used a model containing two steam turbines.

The sparse filterSQP version was used for solving optimisation problems of industrial size including several NLP examples for combined cycle and cogeneration plants with an energy or economic objective function. One of the most complex NLP problems solved was for the profit optimisation for a real cogeneration plant (Gator-Power, 1994) where annual profit was calculated from sales of electricity and steam produced minus expenses in operating and maintenance, fuel, water makeup and power for pumps. The plant model contained nearly 1,500 variables with a similar number of equations and was solved successfully with the filterSQP solver. This cogeneration plant was simulated and optimised without considering supplementary firing (which is sometimes used in this and other cogeneration plants). Chapter 7 presents all the NLP optimisation problems solved.

For the synthesis problems a novel software tool for the solution of MINLP problems with a branch and bound scheme (Fletcher and Leyffer, 1994) was used. This solver has a depth first search and maximal fractional branching (Leyffer, 1998) for the integer part of the problem and the filterSQP method (Fletcher and Leyffer, 1998) for the NLP part. It is called MINLP.BB.

Synthesis examples shown in Chapter 8 aim to find the optimal number and position of heat recovery (HR) exchangers within a HRSG which is part of combined cycle or cogeneration plants. The MINLP model developed considers superstructures for the hot and cold side streams involved in a HRSG; integer variables for the HR exchangers; EO models for every unit operation and logical constraints. The superstructures consider any possibility for splitting, mixing, recycling of streams and for the selection of up to three economisers and superheaters in the HRSG of a CHP plant.

The cost function for the HR equipment was smoothed ⁴ in order to have a continuous and differentiable function for any value of the heat transfer area (including zero area). This smoothed cost function effectively promoted zero area to minimise cost and consequently zero heat load for HR exchangers that do not have to be there as a result of an optimum synthesis solution.

⁴ In fact a smoothing procedure was used for all units having a 'power law' cost function (see e.g. cost models for heat exchangers in Appendix E, Table E.2).
Two synthesis example problems were solved:

- a model for a cogeneration plant where HP steam is produced in a HRSG whose heat coils for superheating steam were synthesised. This model has about 1,200 variables;
- the second synthesis problem is a combined cycle where the heat coils for the economisers and superheaters in the HRSG were synthesised. This model has 3,042 modelling variables, 98 of which are free variables.

1.6 Thesis structure

Literature overview and the areas to explore in this research are presented in Chapter 2. The overview involves the state of the art on the solution methods for design, synthesis and optimisation of utility systems. It also contains a review of the EO approach and large-scale problems reported in the chemical engineering and related literature.

Chapter 3 shows details for the construction of EO models for process streams, for the unit operations present in utility systems and for the energy and economic objective functions. It also shows the MINLP model developed for synthesis problems.

A basic description of the mathematical methods and codes used for simulation, optimisation and synthesis is presented in Chapter 4. This includes a description of the Equation Analyser (Morton and Collingwood, 1998) and the NLAE solver used for simulation (Morton, 1997); the SQP codes used for optimisation (Zoppke-Donaldson, 1995) and (Fletcher and Leyffer, 1998) and the MINLP_BB solver for synthesis (Leyffer, 1998).

Chapter 5 includes details of the infrastructure for EO modelling, simulation, optimisation and synthesis including a description of the modelling package called FMS (Mitchell and Morton, 1996). The chapter presents examples on FMS use to construct simulation and optimisation models, and also provides some details of the interfaces between FMS with optimisation and synthesis solvers, namely the filterSQP/FMS and MINLP_BB/FMS interfaces. Chapter 5 also shows details of the strategy for scaling variables, constraints and derivatives.

Chapter 6 describes the simulation examples with results and discussion. Problems range from simple streams and unit operations to complex examples through which a complete cogeneration plant and a synthesis model for a fixed structure were finally simulated. There is a discussion
of the performance of the sparse NLAE solver.

Chapter 7 contains a description of the optimisation problems solved: the model for a CHP system; a small model having two steam turbines; economic and thermal optimisation of combined cycles; three plant profit optimisation problems for a real cogeneration plant; and a synthesis model for HR exchangers in a combined cycle. Results for the optimised variables as well as a discussion of the solutions and solvers performance are included.

Chapter 8 contains a description, results and solver performance for the two MINLP synthesis problems solved. Chapter 9 has conclusions and recommendations for further work.

Appendices contain:

A rigorous water/steam thermopack;
B equation of state and thermopack for air;
C gas turbine streams thermopack;
D all the unit operations EO models proposed in this research; and
E economic data and cost functions.

In the appendices relevant numerical parameters used for the thermodynamic property packages, for performance equations and for investment and operating costs are included.

1.7 Research contributions

The EO approach for simulation, optimisation and synthesis problems in CHP systems treated in this research provides the following contributions:

○ Proposition, testing and applicability of equation-oriented (EO) mathematical models for the considerable number of process streams, unit operations, investment and operating costs relevant to combined heat and power systems.

○ Some of the original mathematical models proposed for their simultaneous solution include: a rigorous water/steam and air thermodynamic packages, a realistic gas stream
model for gas turbine streams; a model for a commercial gas turbine; a model for an air-cooled condenser and the model of a deaerator among others. The models have twice-continuously differentiable functions.

- Elaboration of Fortran 90 code for the full set of modelling equations and their partial derivative information. Also their interconnection to FMS was contributed.

- Demonstration of the effectiveness of the EO environment, created within our research group, to handle simulation problems as large as 3,022 variables and equations for CHP systems. This shows that our EO environment may be used for larger models not only in utility systems, but in general Process Systems Engineering problems.

- Comprehensive test of novel packages for EO simulation: The EA for identifying free variables and redundant equations and the sparse NLAE solver.

- The proposed models assessed in an extensive study of continuous parameter optimisation of utility systems in an equation-oriented (EO) approach constitute a contribution for the study of CHP systems which are generally analysed in a sequential modular approach.

- The solution of NLP optimisation problems for CHP systems up to industrial size dimensions is a contribution for testing the filterSQP performance in large-scale Process Engineering problems. This is important, since the filterSQP code has been fully tested in solving an extensive set of test problems known as CUTE (Bongartz et al., 1995) used by mathematicians and software developers as in (Fletcher and Leyffer, 1998) and (Lalee et al., 1998).

- A scaling procedure for variables, equations and partial derivatives was added to the filterSQP/FMS interface. So the filterSQP solved fully scaled problems. This allowed efficient solution of NLP optimisation problems.

- An important contribution has been to demonstrate a methodology for generating a starting guess which enables filterSQP successfully to converge large-scale utility systems optimisation models. This involved generating partial solutions for subsections of the total plant using an in-house nonlinear equation solver (Morton, 1997) which were used as starting guesses in simulating successively larger portions of the plant.

The methodology was used to provide a starting point to solve complex optimisation problems. These include a model for a cogeneration plant currently in operation (Gator-Power, 1994) and a MINLP synthesis model with 98 free variables.

- Implementation of an interface between FMS and the software package for solving MINLP problems.
An original MINLP synthesis model for finding the optimal number and position of heat recovery exchangers in a CHP plant was proposed. The MINLP model developed considers: superstructures for the hot and cold side streams involved in a HRSG; integer variables for the HR exchangers; EO models for every unit operation and logical constraints.

The applicability of the proposed MINLP model was tested and demonstrated using two synthesis models. The two synthesis example problems are: a model with 1167 variables for a cogeneration plant and a combined cycle model with 3,042 variables.

The results obtained for the problems solved show that the proposed EO model and the EO environment with the linked mathematical solvers represent a highly efficient approach to the simulation and optimisation of CHP systems. The solution of synthesis problems was not as robust as expected, but may be used for preliminary design stages of CHP systems.
Chapter 2

State of the art overview

Utility systems for providing heat, electrical and/or mechanical power for industrial processes and as public utilities have been of considerable interest over the years. Different approaches for their design, simulation, synthesis and optimisation have been reported and are analysed in Section 2.1. Since we have determined that it is convenient to use an equation oriented (EO) approach for the systems being studied, Section 2.2 contains an overview of this topic in order to present its development and applications in chemical engineering. Section 2.3 includes a review of the work published on large-scale non-linear programming problems with the aim of comparing the reported problems size and characteristics with the utility systems in the EO approach of this research. Here the large-scale problems are described by models with hundreds to thousands of variables having varied and highly non-linear algebraic equations. This literature overview on utility systems, combined heat and power (CHP), the EO approach and large-scale problems leads to the discussion of approaches and identification of the areas for this research as shown in Section 2.4.

2.1 Solution methods for design, synthesis and optimisation of utility systems

Although some of the reported mathematical formulations involve thermodynamics, heuristics and targeting, a separate section (see Section 2.1.2) is presented for purely thermodynamic, heuristic and targeting approaches.
2.1.1 Mathematical formulations

Early work on the solution of utility systems problems by algorithmic methods includes the synthesis of steam and power plants using a linear programming (LP) model to obtain an optimal configuration for a utility system (Nishio and Johnson, 1977); steam balance calculations in a simultaneous approach (Gordon et al., 1978); MILP for the synthesis of steam generation for fixed power and heating demands (Grossmann and Santibañez, 1980) and the use of TISFLO-II, an EO program, for the optimisation of utility generation and supply (Vanmeulebrouk et al., 1982), where the models for two case studies of about 1,000 variables were obtained using measurement data from an actual plant. Their optimisation method is a very simple version of Newton-type method that uses Lagrange multipliers to maximise an objective function using a linearised equations set.

The research of (Papoulias and Grossmann, 1983a) has presented a strategy for the design of utility systems by solving a MILP approach which considers a superstructure with steam and gas turbines. The system is optimised over fixed pressure levels for specified heating and power demands. In (Petroulas and Reklaitis, 1984) a LP strategy is coupled with dynamic programming to optimise a superstructure comprised of gas turbines, steam turbines and process heaters. Their proposed solution is for the preliminary design phase. They require fixed heat sources (from steam) and utility requirements and they get the pressure levels of steam and distribution of steam turbines and steam flows for maximising the work produced. Later (Nishio et al., 1985) solved a synthesis problem of energy supply systems by selecting units for heating and power requirements. Their solution serves for the preliminary selection of equipment in a utility system. It is formulated into a LP model for minimising the use of fuel. (Colmenares and Seider, 1989) present the synthesis of a utility system integrated with a chemical process. A superstructure consisting of Rankine cycles is formulated and solved with a NLP strategy. The model allows for heat and mass integration between adjacent power cycles, which permits the design of complex utility systems. The model is solved in a two-stage algorithm. In an outer loop pressures and temperatures are optimised while in an inner loop flowrates and utilities are optimised.

Multi-objective optimisation by (Clary and Newell, 1990) involve a quantitative measure of the risk of operating against process constraints. They balance this against the operating cost using multiobjective optimisation techniques and propose a trade off between cost and risk. The risk is characterised to reflect both the probabilities and the magnitudes of upsets caused by disturbances. They used a quantitative cost index together with operating costs as objectives.
In multiobjective decision making the non inferior solutions are identified and the selection between them is the best-compromise solution. They use goal programming whose aim is to minimise the sum of the deviations between the objective functions and the goals. They solved a simple problem with two boilers, steam users and a pressure control all considered as blocks without explicit internal performance modelling. Further to that work (Yokoyama et al., 1994) proposed a method for the fundamental design of cogeneration plants, determining equipment capacities and utility maximum demands including minimisation of the annual total cost considering the plant’s annual operation strategy. The sizing is formulated as a NLP program and the operational planing problem is formulated as a MILP. They determined equipment capacities and utility maximum demands as well as the plant’s operational strategy for a given plant structure, utility tariff, energy demand and ambient conditions. As constraints they consider performance characteristics of each piece of equipment and energy balance relationships of each energy flow for average hourly energy demands. They mention that because it takes too much computation time to optimise all the design variables simultaneously they use a hierarchical optimisation method consisting of determining equipment capacities and utility maximum demands at the upper level; and the operational strategy at the lower level; both levels are interconnected by a penalty method. A penalty cost is imposed on the occurrence of virtual energy flows. They use sequential linear programming for the NLP part of the problem and a branch and bound method for the MILP.

Later (Falcetta and Sciubba, 1995) described a modular procedure for the numerical simulation of thermal power plants, taking a combined cycle power plant as an example. They use three matrices: the interconnection matrix (IM), the plant matrix (PM) and the topographic matrix (TM). Starting from a set of input data their Fortran program calculates component by component. They do not mention the level of detail of their calculations. (Seyedan et al., 1995) presented a simulation procedure for the performance of a combined cycle power plant. They validate their procedure by simulating an industrial designed plant with 800 MW capacity. They use manufacturer’s catalogues to get appropriate correlations -not presented in the publication- and they also use heat transfer equations for detailed calculations. Their simulation strategy allows them to finally solve a system of nine non-linear equations with nine variables. Another study using modular simulation includes the thermodynamic simulation of a CHP plant using ASPEN Plus (Ong’iro et al., 1996). The model was validated using field data from two plants with capacity of 105 MW and 150 MW respectively.

Stochastic optimisation has been also used. In (Maia et al., 1995) a combinatorial optimisation approach using simulated annealing (SA) is proposed. They derive flowsheets for systems
to satisfy fixed demands of steam, electricity and mechanical power. Their approach allows
the selection of equipment available in standard capacities by handling discrete variables and
discontinuous cost functions. Their main contribution is that the methods previously presented
do not consider components offered by equipment manufacturers as they do. In their method,
standard equipment is selected from a given set allowing accurate system design and capital
cost by using technical and data cost from manufacturers. They represent equipment capacities
and steam conditions by discrete variables.

SA is a type of local search algorithm that can accept solutions that increase the value of
the objective function, thus avoiding local minima and falling, in principle, into potentially
promising paths. It is based on the physical annealing of solids: the slow cooling of a molten
substance that redistributes the atoms until a low energy state is reached, such as large single
crystals. In rapid cooling or quenching, the result would be a metastable structure with higher
energy, such as a glass or a defective crystal. In the annealing of solids, the goal is to find
some atomic configurations (a feasible solution of a combinatorial optimisation problem) that
minimise internal energy (an objective function). Careful annealing leads to the lowest energy
state (the global minimum) while rapid cooling generates a higher metastable structure (a local
minimum). This method guarantees the global optimum only for an infinite time scheduling,
and for finite time it finds a good suboptimal solution.

In (Maia et al., 1995) the authors require the use of a superstructure embodying several flow-
sheet alternatives to supply the given utility demands. The superstructure should judiciously
limit the search to only suitable solutions. The authors said that SA is suitable for large
systems. They solve a problem with three steam levels with steam conditions to be selected.
And for them, each unit in the superstructure represents a finite set of alternative standard
models, identified by the capacity and the steam conditions on which the unit operates. The
cost of each model is expressed by its present value or equivalent annual cost accounting to
capital and operating expenses. The cost function of a unit presents a constant cost over the
capacity range of each alternative model. For fuel consuming units, the cost of each model is a
nonlinear function of the capacity due to efficiency reduction in partial load. A superstructure
is considered in a similar way to the one in (Papoulias and Grossmann, 1983a).

In the SA approach of (Maia et al., 1995) the total cost is minimised subject to material, energy,
shaft and electricity balances as well as to limits imposed on capacities, steam properties and
structural constraints. They neglect pressure losses in pipes and assign pressure and temper-
ature to the steam levels to the boiler feed water heater, to the condenser and the deaerator.
Their trial and error solution consists of generating a solution vector that activates discrete values for the enthalpy of all streams and for the variables of the units defining a base case. Then the system simulation and the cost function are evaluated. Their numerical example is the synthesis of a utility system of a petroleum refinery of 200,000 BPD capacity which was solved using heuristics in (Nishio et al., 1980) and with MILP by (Papoulias and Grossmann, 1983a). The use of continuous functions as compared with discrete functions for standard capacities of equipment gave to (Maia et al., 1995) a 2.6% error in cost evaluation. They provide information on equipment cost for some nominal capacities.

Other investigations using simulated annealing include the synthesis of utility systems with variable demands (Maia and Qassim, 1997) and the minimisation of annual cost (Wilkendorf et al., 1998) in a synthesis procedure for given utility demands.

Genetic Algorithms (GA) have also been applied to the operation optimisation of a cogeneration system. (Manolas et al., 1996) use a simulation model combined with the GA to maximise the power produced. In GA only the value of the quantity to be optimised is needed, but no derivative information. GA give a final set of good solutions. The simulation model gets the power output of the plant, but its level of detail is not specified.

(Venkatesh and Chankong, 1995) made a decision model for the management of cogeneration plants including models for unit operations considering the thermodynamics of the process and linear calculation of enthalpies. They proposed a MILP model. Another study considering the optimal operation of a steam network (Papalexandri et al., 1996) has a model based on network measurements and data reconciliation techniques. By solving a MINLP model with a generalised Benders decomposition method and GAMS (Brooke et al., 1988) they obtained the optimal selection of furnaces operating at certain conditions. Later a MILP model for the operational planning of utility systems was presented in (Iyer and Grossmann, 1997) where the optimal choice of units operating in each period is determined.

A thermoeconomic optimisation of a cogeneration system in a refinery using thermodynamic analysis reported in (Frangopoulos et al., 1996) proposes a model having 4 degrees of freedom. They also use data collection to obtain correlations for describing steam consumption in steam turbines; gas turbine efficiency as a function of electricity produced; steam produced in HRSG as a function of electricity produced in the gas turbine; and utility consumption of pumps as a function of the pump's flowrate. The optimisation problem is solved with a generalised reduced gradient method. The model is not fully EO since a simulation package is used in the
calculations for determining values of some operating variables.

An approach combining optimisation with a modular simulator was proposed by (Diaz and Bandoni, 1996) where the optimisation algorithm (involving outer approximation (OA) for the MINLP problem) interfaces the simulation code at the nonlinear programming step. For an ethylene plant they handle 4 continuous independent variables, 33 integer variables, more than 200 dependent variables and 48 process constraints. This approach is mentioned here because their plant optimisation includes its corresponding utility system.

A method for the selection of pressure levels in CHP systems by (Marechal and Kalitventezoff, 1997) uses the balanced grand composite curves (GCC) of process and utility streams. By applying Carnot cycle concepts they estimate the potential for power production and the identification of optimal steam pressure levels. Pressure levels and superheating temperatures are derived from the definition of a rectangle in the GCC. Based on the graphical method a MILP is proposed to define pressure and temperatures for the steam network. They obtained the optimum utility and steam flows that minimise the energy cost by producing heat and power. For heat load calculation they use constant specific heat and ideal behaviour for steam turbines power calculation. The water pumping power is neglected.

Recently in (Bruno et al., 1998) a MINLP model for synthesis and operation of utility plants has been proposed. It includes fixed mechanical, electrical and heating demands. The model considers a superstructure similar to the one reported in (Papoulias and Grossmann, 1983a), but with nonlinear equations for equipment cost and for plant performance as a function of enthalpy, entropy and efficiencies. They however consider few variables in their model: flowrates, stream enthalpies and turbine efficiencies. In addition steam header pressures are considered fixed which simplifies the optimisation problem. For discrete fixed pressure values enthalpy expressions are used, thus limiting the whole range of pressure values in which a utility system can potentially operate. Their largest problem solved includes 101 integer variables, 473 continuous variables and 599 constraints.

2.1.2 Thermodynamic, heuristic and targeting approaches

In (Nishio et al., 1980) a thermodynamically oriented approach is proposed for the design of steam systems based on the systematic use of heuristics to decrease the loss of available energy to a minimum. Later the thermodynamic approach by (Chou and Shi, 1987) for the design and synthesis of utility systems was reported. They proposed a method that gives preference
to the heating over the power demands. They solve first the steam cycle then the gas turbine cycle. They suggest that reheating steam systems do not improve the overall thermal efficiency arguing the required large heat-exchange area and the increasing complexity of the system, but they do not prove their assertion. They also mention that a reheat cycle will be of interest to power plant design only when a lot of heat is exhausted to cooling water. However, it is known that at current combined cycle technology reheating systems may reach efficiencies as high as 58.3%, see (Dechamps, 1998).

The work described in (Townsend and Linnhoff, 1981) is focussed on heat and power integration with the process. They introduced qualitative guidelines for positioning heat engines and heat pumps to improve the efficiency of a process having minimum utility requirements for heating and cooling.

Practical guidelines for screening alternatives in plant utility systems expansion are given in (Thomas, 1981). Later, (Peterson and Mann, 1985) gave a set of design guidelines for steam systems for a large chemical complex or oil refinery. They include practical hints for the selection of steam loads, pressure and temperature levels as well as for the selection of steam drivers and for the calculation of steam balances.

The layout selection of heat recovery coils into the HRSG has an important role in the overall performance of CHP systems. Using thermodynamic insights different heat coil layouts have been proposed for HRSG in combined cycle power plants (Stecco et al., 1991). The coils arrangement includes the selection of one or more economisers or superheaters. Targeting methods are related to the use of Pinch Analysis whose concepts were extended by (Dhole and Linnhoff, 1993) to propose a graphical process-utility interface. This representation involves composite curve profiles for a total site (which has several chemical processes). This allows the identification of cogeneration potentials.

Later, (Mavromatis and Kokossis, 1998a) proposed a graphical representation of steam turbine networks that uses linear relations between the steam flowrate and the turbines' power output. They compare the use of the graphical representation with a MINLP formulation (Mavromatis and Kokossis, 1998b) for problems of maintenance scheduling. The MINLP model consists of nonlinear equations relating efficiency to turbines load and was solved with the generalised Benders decomposition (GBD) method. Their larger MINLP model has 1676 continuous variables and 135 binary variables, but no further details are given on the characteristics of the
model. The graphical representation gave similar results compared to the algorithmic method for several examples. However, for two of them the targeting method gave slightly better results compared to the algorithmic method. They conclude pointing that a close integration of conceptual and mathematical models is still needed.

\section{2.2 Equation oriented (EO) approach}

A definition of the sequential modular approach in contrast to the EO approach is given in (Bogle and Pantelides, 1988) and was also presented here in Chapter 1, Section 1.1.2.

A separation of the work published on the EO approach with respect to large-scale nonlinear optimisation cannot readily be done, but in this section an overview of the EO approach to solve problems of any size is presented.

The initial investigations on the EO approach include the work by (Rosen, 1962) for solving simultaneous material balances; a paper by (Umeda and Nishio, 1972) where a comparison between the sequential modular and the EO approach is shown; the solution of flowsheeting problems involving distillation columns in (Westerberg and Berna, 1978) and a book on process flowsheeting by (Westerberg \textit{et al}., 1979).

A review on EO flowsheeting by (Shacham \textit{et al}., 1982) refers to programs like ASCEND (Carnegie Mellon University), FLOWSIM (University of Connecticut) and SPEEDUP (Imperial College). This review concludes the feasibility of using the EO approach for small problems and points out the necessities for large scale EO optimisation. Early applications of SQP in EO flowsheeting include (Locke and Westerberg, 1983) where a reduced space (which is defined by using the number of the degrees of freedom for the problem) method is used to solve medium size problems (with less than 1,000 variables) including distillation columns. The problems have from one to five degrees of freedom.

EO flowsheeting programs use sparse matrix reordering techniques like the ones explained in (Stadtherr and Wood, 1984a) and applied in (Stadtherr and Wood, 1984b) for solving flowsheeting problems. Other desirable attributes of EO flowsheeting systems have been mentioned by (Westerberg and Benjamin, 1985) like decomposition of large systems, variable initialisation, variable and equation scaling and others.
Other equation oriented flowsheeting packages include SEQUEL (Zitney and Stadtherr, 1988); TISFLO-II (Vanmeulebrouk et al., 1982); MASSBAL (Stephenson and Shewchuck, 1986) and the QUASILIN program (Hutchison et al., 1986a).

In the QUASILIN a Newton's method is used for simulation and a Powell SQP method with BFGS for Hessian approximation is employed for optimisation. Examples on the application of the QUASILIN program for problems with up to 460 variables include a system of flash units; a section of an ammonia plant; problems involving distillation columns and a heat exchanger network (Hutchison et al., 1986b).

Later, more experiences on EO chemical process flowsheeting simulation have been reported by (Zitney and Stadtherr, 1988) where different nonlinear equation solvers, problem initialisation and sparse Jacobian generation are addressed. Using a Newton correction-step method implemented in their EO system they solved simulation and design problems the largest being a light hydrocarbon recovery problem with 350 variables. Later, (Kocis and Grossmann, 1989) solved some MINLP problems with an outer approximation/equality-relaxation algorithm, the problems presented include flowsheeting examples with up to 528 continuous variables and a small utility plant retrofit problem (with about 100 variables).

More recently, (Cofer and Stadtherr, 1996) addressed the reliability of nine linear equation solvers used in an EO approach for solving some flowsheeting simulation problems. They mention the necessity of improving reordering and preconditioning schemes when solving large systems of algebraic equations.

Finally, many of the concepts developed in EO optimisation of chemical processes developed over the last few years are presented in a recent process design book (Biegler et al., 1997a).

2.3 Large-scale problems

This is by no means a complete overview on large-scale problems solved with algorithmic methods, but made to clarify the size and characteristics of problems solved under the large-scale category in particular flowsheeting simulation and NLP optimisation problems to which this research is related. Other large-scale applications such as linear programming (Simon and Azma, 1983) and MILP for scheduling batch processes (Bassett et al., 1996) are not considered here. Large-scale optimisation problems are best treated using sparse data structures for derivative
information and include problems with a thousand or more variables (Lalee et al., 1998).

Methods for solving large-scale flowsheeting simulation problems include decomposition of the problem in Newton-Raphson based methods (Westerberg and Berna, 1978); partitioning of the system of algebraic equations in "irreducible subsets" by (Shacham, 1984) and sparse Gaussian elimination with a method to avoid too many non-zeros (fill-ins) during the solution process by (Chen and Stadtherr, 1984). Using a reordering algorithm in sparse systems (Stadtherr and Wood, 1984b) solved flowsheeting problems with up to about 4,700 variables.

Early studies on large-scale NLP problems include (Lasdon and Waren, 1983) where the feasibility of solving large nonlinear optimisation problems with mostly linear constraints is mentioned. At that time solving large chemical process optimisation problems was not a common procedure.

Using a reduced SQP strategy with sparse matrix techniques (Vasantharajan et al., 1990) solved several optimisation problems including non-ideal separation systems, the largest having up to 977 variables. They compared SQP with MINOS (Murtagh and Saunders, 1987) an augmented projected Lagrangian algorithm and found that the reduced SQP needed fewer function evaluations and was less sensitive to the initial guess.

Some other studies reported on the solution of large-scale continuous NLP optimisation problems include an ethylene plant model with 8,500 variables (Rahabar et al., 1990); and NLP equality constrained problems with up to 27,000 variables taken from the CUTE collection (Bongartz et al., 1995) using a trust region SQP algorithm which can use exact second derivative information if available; when it is not a Quasi-Newton approximation is used (Lalee et al., 1998).

Problems on simulation and optimisation of large chemical processes solved with a parallel frontal solver were reported in (Mallya et al., 1997). They use parallel supercomputers to solve optimisation problems for an ethylene plant modelled with 43 units including five distillation columns with around 10,000 variables. A second set of problems for dynamic simulation involved up to around 70,000 variables for interlinked distillation columns. Since a plant model for such an ethylene plant solved in a single CRAY C90 with the standard SPEEDUP program (Aspen Technology, Inc.) took about 18 hours of CPU time they use a parallel algorithm to significantly reduce such computing time.

(Vassiliadis, 1996) used a penalty/modified barrier function (PE/MBF) method for solving large-scale quadratic programming (QP) problems. In this method the solution of an equality
constrained problem is tried followed by an outer iteration where the Lagrange multipliers of the bounds are adjusted. An optimal control convex QP set of problems with up to 20,000 variables and a network flow problem with up to about 6,500 variables were solved. Other approaches to large-scale NLP optimisation problems (Vassiliadis and Floudas, 1997) include the modified barrier function method where the unconstrained nonlinear part of the problem is solved, then the Lagrange multipliers are updated and convergence is checked. The modified barrier function involves the objective to minimise, the Lagrange multipliers and logarithmic terms with information from constraints and for the enlargement of the feasibility region. The problems solved using the modified barrier method include linearly constrained problems with up to 20,000 variables; bound constrained problems with up to 100,000 variables; optimal control problems, the largest being of up to 400 variables; and a molecular potential energy minimisation problem with up to around 8,600 variables.

In addition, large optimisation problems have been solved in the area of real time optimisation (Bailey et al., 1993) where a nonlinear model for an hydrocracker plant in an equation based strategy was solved. Their plant model has 2,891 variables with 10 degrees of freedom which are the setpoints in the plant's control system. They used MINOS (Murtagh and Saunders, 1987) for solving the optimisation problem.

2.4 Discussion of approaches and areas for this research

The state of the art overview on the areas of design, simulation, optimisation and synthesis of utility systems justifies the convenience of studying these systems in a specialised EO approach. Utility systems, in particular CHP plants, are described by highly integrated processes involving multi-loop feed-back connectivities that are best treated in an EO environment where convergence of the flowsheet equations as they move towards the optimum is simultaneous.

Heuristics based methods have the limitation of reducing the energy and capital costs in a very simplified manner, thus limiting too much the search for the lowest total cost optimal solution.

Regarding some of the first mathematical optimisation approaches in utility systems, the solution involving a linear programming approach developed in (Nishio and Johnson, 1977), (Petroulas and Reklaitis, 1984) and (Nishio et al., 1985) also limits the search space for the optimal solution as linear functions are not suitable for realistic modelling of these systems.
For capital cost, continuous functions of equipment capacities have been used, for example, in the work of (Papoulias and Grossmann, 1983a). They adopt a fixed charge function for their MILP strategy. Since traditional exponential cost functions are non differentiable at some points the use of smooth and twice-continuously differentiable cost functions in an EO approach represents a new area for this research.

As seen in the literature survey many of the papers on the EO approach, from early work in EO flowsheeting (Westerberg and Berna, 1978) to more recent research e.g. (Mallya et al., 1997) in EO simulation and optimisation, mainly consider flowsheets involving distillation columns.

It was also found that problems for CHP systems with commercial gas turbines have been solved using modular simulation (Falcetta and Sciubba, 1995), (Seyedan et al., 1995), (Ong‘iro et al., 1996), whose use is limited for highly integrated processes.

Early attempts at using an EO approach specifically on utility systems (Gordon et al., 1978) are limited to the simple calculation of steam balances; and to the optimisation of utility generation and supply (Vanmeulebrouk et al., 1982) where simple models were obtained using measurement data from an actual plant, and a very simplified optimisation method was used. More recent EO approaches to these systems involve a MINLP model with few variables and simplifications like the discrete specification of operating pressure levels (Bruno et al., 1998) for fixed heat and power demands that make this approach to be less general and more easy to solve than a more extensive EO model.

Thus, a specialised model for an EO approach to utility systems of industrial size is a new challenge. The model may provide extensive units and streams information (like in sequential modular simulators) through the many variables involved in a new EO environment. The modelling task for the CHP systems includes coupling closely to the sort of information required by the optimiser (e.g. smooth twice-continuously differentiable modelling equations) for the successful application of the optimisation code. A realistic EO model for a CHP system includes many variables and strong nonlinearities in the majority of the constraints. As mentioned most of the techniques used so far have limited their nonlinear capability to few constraints, but utility systems have equipment with many nonlinearities producing large-scale problems difficult to solve.

EO modelling, implementation and testing of the very large amount of process streams and unit operations as well as different criteria for optimisation (like energy efficiency and economics)
for CHP systems produces large-scale flowsheeting problems which are the area of interest in this research. The resulting simulation, optimisation and synthesis problems require efficient sparse solvers and the implementation of suitable initialisation strategies for giving appropriate values to the many modelling variables for robust and efficient convergence of the solvers.

The performance of any gradient-based algorithm is strongly dependent on the accuracy of the derivative calculations for the objective and constraint functions (Biegler, 1992), so we propose the provision of exact analytical derivatives, which have not always been used in other investigations when solving large-scale optimisation problems.

Some models can be rigorously proposed combined with simplified ones and as the size and/or complexity of the problems grow, we decide whether the use of simplified models may substitute for exact models in some sections of the plant. That is because increased simplicity in modelling can reduce effectiveness while on the other hand too many considerations can reduce robustness of the solution. The explicit treatment of nonlinear models for better modelling and smooth continuously differentiable equations is a challenge to test the robustness of modern optimisation codes when solving industrial size problems.

The use of a rigorous EO thermodynamic package for water/steam and air streams in the context of CHP plants additionally represents an interesting area of research since EO approaches normally deem these stream properties to be obtained by simplified methods.

There is no single nor global technique which rigorously ensures a global optimum solution for the large, complex nonlinear and discontinuous optimisation space characteristic of plant utility systems.

Robust modern optimisation codes for large-scale nonlinear problems have been fully tested in solving mathematical test problems (Fletcher and Leyffer, 1998), (Lalee et al., 1998). New MINLP solvers like the MINLP_BB (Leyffer, 1998) which is linked to the filterSQP code (Fletcher and Leyffer, 1998) used here has also proven robustness in solving mathematical test problems. Other MINLP algorithms (Skrifvars et al., 1998) were used to solve problems with a large number of variables, but small variety and complexity of the objective and constraint functions. So, another new area of research is to test the proposed codes (See Chapter 1, Section 1.1.3) for the solution of industrial size CHP simulation, optimisation and synthesis problems in a new EO environment recently created within our research group.

The NLP optimisation codes for this research (as any other current available NLP solver) do
not assure a rigorous guarantee for the global optimal solution, which can only be provided for the case when the nonlinear functions are convex. Since a realistic model for CHP plant necessarily involves non-convex functions, no global minimum is guaranteed, but solutions that are relevant for practical applications may be obtained. This is because we combined rigorous and realistic models in our EO approach.

From the literature reviewed it appears that the synthesis problem in utility systems has been solved using LP, MILP, MINLP, GA and SA considering systems in the overall but generally simplified context. Thus, based in a fundamental EO model with many variables and constraints, different subsections or whole CHP systems may be synthesised by solving the resulting MINLP model. All the research reviewed concentrates on developing relatively simple, low dimensional representations with few variables in the process model that render the optimisation problem relatively easy to solve and understand. Some strategic areas within CHP systems, like the optimal synthesis of heat recovery coils in the HRSG, have been unexplored using algorithmic methods. Thus the application of the proposed EO environment for producing a synthesis model for the generation of steam in HRSG within the context of a whole plant performance is another area to investigate.

In utility systems the reported synthesis models involving a superstructure generally involve simplifications like fixed heat and power demands, and isothermal mixing of streams defining a superstructure. The application of fundamental EO models may easily create superstructure models considering the exact calculation of mixing temperature and the capability to have any free variable within the plant model. This is a new challenge in EO approach to utility systems.

Because of its level of applicability and industrial interest, the research is focused on CHP plants in which natural gas drives gas turbines and steam at different pressure levels is produced in a HRSG. The steam can be exported or used for the production of power in steam turbines. Finally, unexplored areas in the use of modern algorithmic methods include the fundamental and extensive EO modelling for utility systems of industrial size, including plants in operation. The resulting EO approach applied to the simulation, NLP optimisation and synthesis of CHP systems proposed in this research is expected to be an original and useful work for the study of these systems.
Chapter 3

Equation oriented models for CHP systems

There is much industrial interest in utility systems, in particular combined heat and power (CHP) systems which are used in the production of electricity and process heat and/or mechanical power from the same primary energy source. For this reason and in order to use the EO approach to simulation, optimisation and synthesis a fundamental model for CHP systems was developed. We are interested in CHP plants containing steam turbines and gas turbines fuelled with natural gas. A typical CHP plant is shown in Fig. 3.1. In steady state, the EO model for a process plant should include a set of independent algebraic equations for every single process stream and unit operation.

In the equation oriented (EO) modelling approach described here, we propose a fundamental model for process streams and unit operations describing realistic heat and power systems.

The EO models for describing CHP systems are:

1. water/steam streams
2. air streams
3. gas turbine streams
4. steam turbine
5. gas turbine with and without steam injection (described by compression section, combustion section and expansion section models)
Figure 3.1: A typical CHP plant.

6. heat recovery equipment (which is part of a heat recovery steam generator (HRSG))

7. steam drum

8. deaerator

9. air-cooled condenser

10. pump

11. shell and tube heat exchanger

12. mixer/splitter (multi-component streams)

13. mixer/splitter (single component streams)

14. compressor

15. heater/cooler

16. valve
A description of the construction of fundamental models for process streams is given in Section 3.1 and details of them are shown in Appendices A to C.

The logic for the construction and some details of unit operation models are presented in Section 3.2. Appendix D shows every single unit operation model developed in this research. The rest of this chapter includes a description of the models used for simulation, optimisation and synthesis and the MINLP model.

3.1 Process streams models

Each type of process stream is a set of variables and equations. Basic details are given in (Morton and Rodríguez-Toral, 1997) and the main features of models are outlined below.

The EO model includes a rigorous physical description of water/steam and air process streams as well as a realistic model for gas turbine streams.

Some of the equations in the water/steam model are non-smooth. A special smoothing procedure is used to approximate these with smooth polynomials which the optimisation code can handle.

For process streams, the model uses a set of thermodynamic subroutines involving twice-continuously differentiable equations for the physical properties relevant in heat and power systems. First and second derivatives of these quantities are returned by the physical property subroutines for use when solving optimisation problems.

It should be mentioned that the initial rigorous water/steam and air stream models consider the set of equations and variables shown in the next two sections. Later, for some simulation problems (Chapter 6), for all the optimisation problems in Chapter 7 (except the one in Section 7.1) and for the synthesis problems (Chapter 8) it was necessary to add an additional equation for a new variable, the stream specific volume ($v$).

In water/steam streams $v$ was needed for a cost correlation for make-up water and may be useful if further models involving the use of $v$ would be added. Air streams needed $v$ for the fan power calculation in the air-cooled condenser model.
3.1.1 Accurate water/steam stream models

There are several difficulties in establishing a mathematical description for these streams, because the model should be able to handle different phase possibilities which inevitably involve a non-smooth function (Morton, 1994a). Careful modelling is needed so that the equations have the same structure in different phase cases.

The set of variables for a water/steam stream is chosen to be:

- \( F, P, h, H, T, s, \phi, q, T_s, h_f, h_g \) (11 variables).

These are respectively: mass flow, pressure, specific enthalpy, enthalpy flow, temperature, specific entropy, vapour fraction, stream quality, saturation temperature, enthalpy of saturated liquid and enthalpy of saturated vapour.

Only three of this set (e.g. \( P, h, F \)) are needed for a full description of the stream. The others are useful since they appear in various unit operations models, or may be used to define other water/steam stream variables.

The dependent variables are defined by 8 equations:

\[
\begin{align*}
H - hF &= 0 \\
h - [\phi h_V(T, P) + (1 - \phi) h_L(T, P)] &= 0 \\
s - [\phi s_V(T, P) + (1 - \phi) s_L(T, P)] &= 0 \\
P - P_{sat}(T_s) &= 0 \\
\phi + aq &= b \\
(h_g - h_f)q - h_g + h &= 0 \\
h_f - h_f(T_s) &= 0 \\
h_g - h_g(T_s) &= 0
\end{align*}
\]

Here, \( h_L, h_V, s_L, s_V, h_f, h_g, \) and \( P_{sat} \) are physical property correlations as defined below.

All the above equations are twice continuously differentiable smooth functions except equation (3.5) which relates the vapour fraction to the stream quality (Morton, 1994a) and in which values for the constants 'a' and 'b' depend on the phase:

---

1 In this set of equations the subscript \( V \) and \( L \), are for vapour and liquid phases respectively.
\[ a = 0, \quad b = 0 \quad \text{for liquid,} \]
\[ a = 1, \quad b = 1 \quad \text{for a saturated two-phase mixture,} \]
\[ a = 0, \quad b = 1 \quad \text{for vapour.} \]

Since equation (3.5) is a non-smooth function, in order to be able to use that function in our NLP optimisation problems it was necessary to use a smoothing procedure for the function in the regions where it is non-smooth, i.e. in the region close to saturated vapour \((\phi \approx 1.0)\) and in the region close to saturated liquid \((q \approx 1.0)\), see Fig. 3.2.

![Figure 3.2: Diagram for \(\phi\) as a function of \(q\).](image)

By fitting a polynomial to equation (3.5) in the region where the function is nonsmooth, the following polynomial was found for the region close to saturated vapour:

\[
\frac{1}{16} \frac{q^4}{\varepsilon^3} - \frac{3}{8} \frac{q^2}{\varepsilon} - \frac{1}{2} q + 1 - \frac{3}{16} \varepsilon
\]  

(3.9)

where \(\varepsilon\) is a small value \(^2\) that defines the maximum deviation of the fitted polynomial from the exact definition of \(\phi\).

For symmetry, in the region close to saturated liquid \((q \approx 1.0, \text{see Fig. 3.2})\) taking 1.0 minus equation (3.9) but using \((1 - q)\) instead of \(q\) we got the following polynomial:

\[
\frac{1}{2} - \frac{1}{16} \frac{(1 - q)^4}{\varepsilon^3} + \frac{3}{8} \frac{(1 - q)^2}{\varepsilon} - \frac{1}{2} q + \frac{3}{16} \varepsilon
\]  

(3.10)

The last two polynomials smoothed equation (3.5) thus allowing its use in NLP optimisation problems.

\(^2\) in our experience \(\varepsilon = 2.0 \times 10^{-5}\) worked well.
Mathematical expressions that constitute the accurate description of this stream are given in a physical properties package (Morton and Rodríguez-Toral, 1997). Accurate nonlinear functions along with their first and second partial derivatives were constructed for:

- water enthalpy, $h_L(T, P)$,
- superheated steam enthalpy, $h_V(T, P)$,
- water entropy, $s_L(T, P)$,
- superheated steam entropy, $s_V(T, P)$,
- enthalpy of saturated liquid, $h_f(T_s)$,
- enthalpy of saturated vapour, $h_g(T_s)$, and
- saturated vapour pressure, $P_{sat}$.

These functions and derivative information are calculated in subroutine calls and used in equations (3.1-3.8). Appendix A shows the accurate expressions for those physical properties.

### 3.1.2 Accurate air stream models

Air is needed in some of the utility systems optimisation examples and in the air-cooled condenser present in one of the synthesis problems. We consider air as a single pseudo component, which is a convenient simplification when no chemical reaction occurs from its molecular constituents (i.e. $N_2$, $O_2$, etc.).

For the utility systems examples presented here, air is in the gas phase only.

The stream description contains 6 variables (Morton, 1994a):

- $F$, $P$, $h$, $H$, $T$, $s$.

These variables are respectively: mass flow, pressure, specific enthalpy, enthalpy flow, temperature and specific entropy.
Once again there are 3 independent variables and 3 equations are needed to define the stream type:

\[ H - hF = 0 \]  \hspace{1cm} (3.11)
\[ h - h_a(T, P) = 0 \]  \hspace{1cm} (3.12)
\[ s - s_a(T, P) = 0 \]  \hspace{1cm} (3.13)

where the subscript 'a' refers to air thermodynamic properties. Again the specification of two intensive variables, like \( P, T \) (or \( h \)) and one extensive variable, like \( F \), allows the simultaneous solution of the above 3 nonlinear equations to describe fully an air process stream.

Since there is no reaction and the air is not near condensation, we use a gas equation of state for the accurate calculation of air enthalpy and entropy, \( h_a(T, P) \) and \( s_a(T, P) \). The Beattie-Bridgeman equation of state was selected because it is reliable at high pressures, except when the critical density is exceeded (Reid et al., 1987), and thus suitable for utility system problems at practical operating conditions. Another advantage of this equation of state is that after a series transformation it can be solved for the specific volume ‘\( v \)’ explicitly (Lee, 1954). Details are in Appendix B.

### 3.1.3 Gas turbine streams models

As gas turbines are modelled, the following gas streams should be considered:

- Air (\( N_2, O_2 \) mixture).
- Gas fuel (\( CH_4, C_2H_6, C_3H_8, n-C_4H_{10}, n-C_5H_{12} \) mixture).
- Exhaust gas (products including combustion and dissociation reactions).

The stream definition is similar to the other streams modelled in our EO approach (Morton and Rodríguez-Toral, 1997), and contains \( N + 6 \) variables (where \( N \) is the number of components for a given gas stream). They are:

\[ F, H, T, P, h, s, y_i, i = 1, \ldots, N, \]

respectively molar flow (which is convenient for the combustion process modelling), enthalpy flow, temperature, pressure, molar specific enthalpy, molar specific entropy, and mole fraction.
Since the Phase Rule requires there to be $N + 2$ independent stream variables, there must be 4 modelling equations associated with a gas stream. These may be written as:

\[ H - hF = 0 \]  
\[ h - h_{\text{stream}}(T, P, y_i) = 0 \]  
\[ s - s_{\text{stream}}(T, P, y_i) = 0 \]  
\[ \Sigma y_i - 1 = 0 \]

In a gas turbine using natural gas we have combustion of fuel at a high air/fuel proportion (more than 92% mole fraction is air in the air/fuel mixture) and the combustion products are 'like hot air' since they have more than 76% mole fraction of $N_2$ and more than 14% mole fraction of $O_2$. On the other hand the use of ideal models for air properties predicts within 1% difference the real models at high temperature and pressure (Irvine and Liley, 1984). Thus, the application of an ideal model (considering temperature and composition effects only) for gas streams in gas turbines at high temperatures and pressures from 1 to 30 bar (operating range of modern gas turbines) is satisfactory. The prediction of our full model for a real cogeneration plant at Florida, U.S.A. (see Chapter 6, Section 6.6.4) confirms this statement. Thermopack for gas streams present in gas turbines is presented in Appendix C.

### 3.2 Unit operations models

In the Equation Oriented (EO) modelling approach described here, a fundamental model is constructed based on balance and performance equations for realistic heat and power systems. Details of its initial development have been reported (Morton and Rodríguez-Toral, 1997) and an extended version was applied to some complex simulation and optimisation examples (Rodríguez-Toral et al., 1999b).

We develop mathematical relationships for material balances and energy balances, momentum balances (or pressure relationships) and performance equations for each equipment type relevant to CHP systems.

The steady-state unit operations models used in this work were developed from fundamental principles to promote process understanding and confidence in the models. They also ensure that the modelling equations for a single unit operation or a whole system are independent.

Each model was written so as to be solvable given fully specified feed streams and appropriate
unit design variables (e.g. isentropic efficiency in the case of steam turbines). There are as many equations as needed to obtain the independent variables in each material outlet stream and any dependent local variables associated with the unit. The models have the required variables for connecting streams and for the unit's performance.

For any unit operation, the total number of variables involved in a certain unit operation minus the number of modelling equations is called the number of degrees of freedom. Process equipment models include the determination of the number of degrees of freedom which in simulation problems, were fixed. The models were designed to be solved stand-alone and in a network.

Each unit operation model considers:

- Material balance equations,
- Energy balance equations,
- Momentum/pressure relationships,
- Performance equations.

Along with the performance equations we propose realistic models in accordance with current design practice e.g. for waste heat recovery equipment (Ganapathy, 1991), for deaerators (Ketten, 1986) and for other equipments. Models for unit operations in CHP systems are fully described in Appendix D.

3.3 Simulation models

EO models for the simulation of single streams, unit operations, plant sections and whole CHP systems were constructed by selecting the relevant streams and unit operations models. Such EO models defining our simulation problems result in sparse systems of nonlinear algebraic equations that in general have more variables than equations resulting in the degrees of freedom.

In a sparse system every modelling equation has a small fraction of the total number of variables defining the model. This is because variables and equations defining a whole flowsheet are setting up for their simultaneous solution. For example, a unit mass balance equation has only few variables with respect to the total number defining a plant model.
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The provision of suitable specifications for the degrees of freedom and the solution of the resulting sparse nonlinear algebraic equations system, constitute the EO simulation problems.

Chapter 6 shows the actual simulation models and results for the many problems solved in CHP systems.

3.4 Optimisation models

The optimisation of utility systems involves an objective function for minimising energy consumption or capital and operating costs subject to the constraints given by the system model and by bounds on variables.

As the objective function (O.F.) and many of the modelling equations are nonlinear the problem must be formulated as a nonlinear programming (NLP) optimisation problem which can be represented as:

$$\min \ O.F. \ = \ f(x)$$
subject to:
$$c_i(x) \ = \ 0.0$$
$$x_L < x < x_U$$  \hspace{1cm} (3.18)

where \(c_i(x)\) is the set of constraint functions and \(x_L, x_U\) are lower and upper bounds on the modelling variables. A relevant objective function is optimised subject to the constraints given by all the modelling equations and by the bounds on variables. For heat and power systems these bounds are applied to temperatures, pressures, power produced by steam turbines, etc. The objective function is optimised simultaneously with the satisfaction of the constraints as the continuous free variables reach their optimum values.

Two types of objective function were optimised as detailed in the next sections.

3.4.1 Energy efficiency objective functions

In some of the optimisation problems solved in Chapter 7, the energy efficiency was maximised. In general this was given by the plant's thermal efficiency, \(\eta_h\):

$$\eta_h = \frac{\sum W_i}{\sum Q_j}$$  \hspace{1cm} (3.19)
where $W_i$ is the gas and or steam turbines power output and $Q_j$ is the heat given to the CHP plant.

### 3.4.2 Economic objective functions

The first NLP optimisation problem (see Chapter 7, Section 7.1) has a simple economic objective function given by the cost of purchased electricity and steam generation. This problem was solved in the initial stage of the project using a SQP algorithm with a 'tolerance-tube' approach (Zoppke-Donaldson, 1995) to decide whether to accept a step from the QP subproblem. More complex NLP optimisation models solved using FMS (the modelling system) and the NLP optimisation code, filterSQP (Fletcher and Leyffer, 1998) use a general economic objective function as detailed below.

**General economic objective function**

The economic objective function is the profitability measure for the optimisation problems treated here. Economic optimisation problems are more complex than the energy use minimisation problems since they involve capital and operating costs as well as revenues. A general economic objective function was developed for use in complex optimisation and synthesis problems.

In many real optimisation problems the objective function has a 'cash flow', involving income and expenses (Edgar and Himmelblau, 1989). In the economic optimisation problems treated here a fixed annual cash flow is considered. More detailed economic analysis would imply the use of a variable annual return from an investment. For instance, the incremental profit from a new plant facility will tend to be lower in the early stages of its operating life, due to high start-up expenses. After that, evolutionary improvement in operating conditions would allow annual profits to reach some peak. Nevertheless, in the later stages of the plant life earnings would decrease because of equipment replacement, failures, shutdowns, etc. Although not implemented here, a more detailed economic analysis may be easily implemented in this EO approach.

The economic objective function considers:

- **Capital Costs.** Which is the cost of equipment or structures with useful life of more than
one year.

- **Operating Costs.** Occur in a yearly basis and are related to the cost of electricity, fuel, make-up water, etc.

- **Profit.** From selling steam and electric power produced by gas and steam turbines.

All of them should be expressed in the same units, e.g. U.S. $/year.

Our general economic objective function involves capital costs for the purchase price of the equipment, operating costs and profit terms for a return on the investment. In this problem it is possible to optimise design variables and operating conditions. The formulation of this sort of objective function presents the greatest conceptual difficulty.

The capital costs involve equipment with a lifetime of “T” years. The funds to purchase and install the plant can be (hopefully) borrowed from a bank and paid back in “T” annual installments.

In order to obtain annualised capital costs (in $/year) the repayment multiplier “r” is defined as the fraction of installed cost to be paid each year to the bank and is obtained from (Edgar and Himmelblau, 1989),

\[
r = \frac{i(1 + i)^n}{(1 + i)^n - 1}
\]  
(3.20)

where “i” is the interest rate (10% - 15% is reasonable (Edgar and Himmelblau, 1989)) and “n” is the number of years to pay back the investment.

For a quantity of borrowed money “B” the fixed annual capital charge “Ch” is,

\[
Ch = r B
\]  
(3.21)

The maximisation of profit involving capital cost is related with a more complex design problem and involves capital and operating costs as well as revenues. This kind of optimisation problem was tackled using a general economic objective function.

The measure of profitability to be maximised was chosen to be the net present value (NPV), because among other methods used in economic analysis (like payback period and Internal Rate of Return) NPV gives more realistic results for a wide variety of cases (Edgar and Himmelblau, 1989).
The selected profitability measure (objective function) is an explicit function of cash flow and capital investment \((I_0)\). The profitability measure thus can be expressed as a function of independent variables.

An objective function may be proposed as the NPV (in $) of before-tax profits for a constant annual cash return \(\text{"CF"}\) over \("n\) years and expressed as,

\[
NPV = \frac{CF}{r} - I_0
\]  \hspace{1cm} (3.22)

where \(\text{"CF"}\) is the annual profit before taxes or (credit for selling electricity and/or steam minus expenses for buying external utilities) and \('r'\) is calculated for a selected interest rate \("i\) and project life \("n\) from equation (3.20).

For most industrial optimisation problems fairly uniform cash flows occur, so that optimising the NPV is acceptable (Edgar and Himmelblau, 1989). The need for an explicit objective function also favours the selection of a NPV-type for the economic optimisation of utility systems.

We could do the minimisation of investment and operating costs as an addition of terms, but the maximisation of profit (given by the NPV) is a more satisfactory measure from the economic point of view.

As mentioned, our economic objective function is to maximise the NPV. Using equation (3.22), we can write,

\[
r \cdot NPV = [CF - r \cdot I_0]
\]  \hspace{1cm} (3.23)

Thus, our general economic objective function \((O.F.)\) is expressed as,

\[
O.F. = - \left( \left(\text{Op. Incomes} - \text{Op. Expenses} \right) - r \left(\text{Capital Costs} \right) \right)
\]  \hspace{1cm} (3.24)

where \(O.F.\) considers annualised costs and is expressed in $/yr. \(\text{Op. Incomes}\) may come from selling electricity and steam. \(\text{Op. Expenses}\) are due to external utilities, operating and maintenance. \('r'\) is obtained from equation (3.20) and the term \(\text{Capital Cost}\) involves any piece of purchased equipment in CHP systems.

In equation (3.24) the first \textit{minus sign} on the right hand side is introduced because our optimiser minimises an objective function subject to a set of constraints and we would like to maximise the \textit{net present value} (from which we derive the objective function).

For convenience all the economic data in equation (3.24) should be expressed in a common
year of reference. It was decided to express costs in 1997 prices. All the economic data (see Appendix E) were obtained from the open literature and expressed in 1997 costs.

For the complex economic optimisation problems of this research, the installed equipment costs for 1997 ($C_{1997}$) is obtained from,

$$C_{1997} = \text{Inst}_F \left( C_x \right) \left( \frac{CE_{Ind.1997}}{CE_{Ind.x}} \right)$$  \hspace{1cm} (3.25)

where 'Inst$_F$' is the equipment installation factor, 'C$_x$' is the cost of the equipment at year "x" and 'CE$_{Ind.1997}$', 'CE$_{Ind.x}$' are the "Chemical Engineering Plant Cost Index" at year 1997 and at year "x" respectively (Edgar and Himmelblau, 1989).

The equipment "Installation Factor" (Inst$_F$) used for the main pieces of equipment involved in our utility systems is presented in Appendix E. It should be mentioned that some of the costs investigated are for installed equipment (e.g. shell and tube heat exchangers) and some others are for 'purchase costs' (e.g. Air Coolers). Therefore Inst$_F$ was used only for equipment whose ‘purchase cost’ was available. All equipment cost however were expressed in 1997 costs.

Appendix E also shows the operating costs used for utilities and the capital cost functions of equipment.

The proposed 'General economic objective function' (O.F.) -equation (3.24)- used in complex optimisation and synthesis problems (shown in Chapters 7, 8) was programmed for use in the modelling system (FMS). Among the characteristics of this general economic objective function we have:

1. The user could select a scale factor for the O.F.

2. For a given utility system the user could select,
   - number of steam turbines
   - number of pumps
   - number of air coolers
   - number of fans consuming power (for air coolers)
   - number of steam pressure levels
   - whether the steam is going to be sold or bought (in some of the optimisation and synthesis problems steam is sold)
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- number of heat loads given by burning fuel
- number of shell and tube heat exchangers
- the value of the "Chemical Engineering Plant Cost Index" for the common economic base year (in this case 1997)
- the capital recovery factor, "r" used to get the annualised fixed capital cost of equipment
- number of deaerators
- number of gas turbines

On the other hand, in order to use successfully exponential equipment cost functions in NLP optimisation problems it was necessary to develop smoothed equations in the region near discontinuity. An example of exponential cost functions is the cost function for shell and tube heat exchangers (Ahmad et al., 1990),

\[ C = 30.8 + 0.75A^{0.81} \]  \hspace{1cm} (3.26)

where 'C' is the exchanger cost in k$ (thousands of U.S. Dollars) and 'A' is the heat transfer area in m². This kind of cost functions have a fixed charge term (in this case 30.8 k$), an independent variable (in this case 'A') multiplied by a constant and a fractional power (0.75 and 0.81 respectively). Equation (3.26) has a first derivative that goes to infinity as \( A \to 0 \).

We have developed a smoothing procedure for discontinuous cost functions. This procedure requires the supply of a "cutoff" from which the smoothing is done.

The smoothed cost function (below the "cutoff" value \( A_{cut} \)) for shell and tube heat exchangers has the form:

\[ C_s = b_1 A + b_2 A^2 + b_3 A^3 \]  \hspace{1cm} (3.27)

where \( b_i \) = 1, \ldots, 3 are chosen to give a smooth continuous (twice differentiable function at \( A = A_{cut} \). The smoothing procedure consists of equating the proposed polynomial, equation (3.27), to the original cost function, equation (3.26), and the same is done for their 1st and 2nd derivatives. The solution of the resulting system of equations gives the values of \( b_i \).

Thus smoothed cost functions were used for:

- shell and tube heat exchangers
Maximisation of profit for existing CHP plants

In utility systems optimisation where the plant is already installed we can use our general economic objective function. In this case the objective function is to maximise the net profit obtained by selling electric power and steam minus the annualised cost of purchasing external utilities like fuel, make-up water and other expenses. This kind of problem can be called a "supervisory control" problem (Edgar and Himmelblau, 1989), which arise when capital costs are a fixed sum, because the equipment is already in place. Since this type of optimisation problem considers an existing plant then we will consider the annualised capital costs as a fixed sum. Thus no Capital Costs term is considered in equation (3.24) and the annualised net profit for existing CHP plants is expressed as:

\[ O.F. = - \left( \text{Op. Income} - \text{Op. Expenses} \right) \]  

(3.28)

where,

\[ \text{Op. Income} = \text{Sales of Net Power produced} + \text{Sales of Steam produced} \]

and,

\[ \text{Net Power produced} = \text{Gas and steam turbines output} - \text{pumping power} \]

\[ \text{Op. Expenses} = \$ \text{Fuel} + \$ \text{demineralised makeup water} + \$ \text{Operating and Maintenance} \]

In chapter 7, Section 7.6 we present three complex optimisation problems for the net profit optimisation of an existing cogeneration plant at the University of Florida. There, the objective function (O.F.) is to maximise the annual net revenue obtained by selling electric power and steam minus the annual cost of purchasing the external utilities and also the operating and maintenance costs.
3.5 MINLP synthesis model

CHP plants are considered in the MINLP model. These plants may have a gas turbine; a HRSG producing steam at different pressure levels; a deaerator; an air-cooled condenser; steam turbines and auxiliaries.

The synthesis problem consists in finding an optimal process flowsheet by solving a model having continuous and integer variables. The resulting MINLP problem can be represented as:

\[
\begin{align*}
\text{min. } O.F. & = f(x,z) \\
\text{subject to :} & \\
\begin{align*}
c_i(x, z) & = 0.0 \\
x_L & < x < x_U \\
z & \in \{0, 1\}
\end{align*}
\end{align*}
\] (3.29)

where objective function \((O.F.)\) for the problems in this research is derived from our general economic objective function combining investment and capital cost as well as profit from selling electricity and steam. \('c_i(x, z)'\) is the set of constraint functions modelling process streams, unit operations and logical relationships involving just integer variables or relating integer to continuous variables. \('z'\) is a vector of \(\{0, 1\}\) integer variables denoting the existence \((z = 1)\) or not \((z = 0)\) of a process unit. For the problems solved here an integer variable is assigned to heat recovery (HR) exchangers. \('x_L, x_U'\) are lower and upper bounds on the continuous modelling variables like temperatures, pressures, power produced by steam turbines, etc.

The MINLP problem involves the representation of alternatives in a hyperstructure (Floudas, 1995) where all process alternative structures are considered.

The general structure of the MINLP synthesis models can be represented as in Fig. 3.3, where an economic objective function (see Section 3.5.1) is optimised subject to the constraints given by the plant model. The constraints are divided into those involving only continuous variables (as models in Sections 3.1 - 3.2), the logical constraints having integer variables (see Section 3.5.4) and bounds on variables.

The synthesis problems presented in Chapter 8 consist of obtaining the optimal arrangement of heat recovery (HR) coils and the calculation of relevant continuous free variables in the context of a whole CHP plant model. The objective function combines the incomes from
annual electricity and steam sales and expenses from annualised cost of external utilities and installation of purchased equipment.

One hot stream (the gas turbine exhaust) must be cooled through an undefined number of HR exchangers constituting the HRSG. In the synthesis problems shown in Chapter 8 we do not have fixed flows nor inlet and outlet temperatures for the different streams defining the hyperstructure (described in Section 3.5.2). We only have the initial gas turbine exhaust conditions that are calculated in the proposed EO model by giving the required specifications defining the nominal gas turbine performance. The hot and cold end temperature differences $DT_h$ and $DT_c$ in heat exchangers will be also optimally found by setting appropriate bounds on this variables throughout.

The problem is to derive a HRSG configuration with optimum total cost. Since we have an accurate stream model the enthalpy is not linear as in other synthesis models using superstructures (Floudas et al., 1986).

Based on fundamental rules for superstructure creation, a flowsheet is specified and a solution containing optimal structure and continuous variable optimisation is obtained by solving the MINLP model proposed in this research. The MINLP model contains the relevant plant model used for the optimisation problems, integer variables for the heat recovery exchangers in a HRSG and logical constraints.

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3 defined for LMTD calculation, see Appendix D, Section D.3
3.5.1 Objective function for MINLP problems

The general economic objective function proposed for NLP optimisation problems (see equation (3.24)) considers explicitly the individual equipment cost functions. This means that each equipment model does not include its cost function within the unit model. For HR exchangers in synthesis models the equipment cost function was selected as an equation within the unit model. The cost function for HR exchangers (whether economiser, evaporator or superheater) has the same form, e.g. for superheaters is expressed as (Wells and Rose, 1986):

\[ C = 2.75 A^{0.5} \]  \hspace{1cm} (3.30)

where 'C' is the HR exchanger cost in k$ and 'A' is the heat transfer area in m².

Thus the general economic objective function (equation (3.24)) is used for synthesis models as,

\[
O.F. = - \left[ \left( \text{Op. Incomes} - \text{Op. Expenses} \right) - r \left( \text{Capital Costs} \right) \right] - r \cdot \sum_{j=1}^{N_{HR}} C_{HR,j} \]  \hspace{1cm} (3.31)

where \( N_{HR} \) is the total number of HR exchangers in the HRSG, \( C_{HR,j} \) is the installed cost of HR exchangers and 'r' is given by equation (3.20).

The stated objective function involves:

- 'Op. Incomes'. Obtained from the gas and steam turbines’ electric power and from the price of the steam produced at pressures other than the low pressure (LP) level.

- 'Op. Expenses'. The operating expenses involving cost of fuel for gas turbines, cost of pumping power, fan power cost for air coolers and operating and maintenance cost.

- 'Capital Costs'. For the major pieces of equipment as given in Appendix E.

3.5.2 Derivation of superstructures

The basic ideas for the derivation of the network superstructure for the HRSG were adapted from concepts given in (Floudas et al., 1986) and (Floudas and Ciric, 1989). There a network superstructure was derived for the synthesis of heat exchanger networks.
In the superstructures derived here alternatives for splitting, mixing and bypassing streams through HR exchangers are considered. However, we do not have the minimum number of units predicted by the MILP transshipment model, nor the initial and target temperatures for the different streams as input data as in (Papoulias and Grossmann, 1983b), but all of these variables are simultaneously optimised within appropriate bounds on variables.

In the CHP plants modelled for synthesis problems the low pressure (LP) steam level is just for deaeration purposes and other steam levels are produced for selling or for power generation. LP steam is produced saturated from a LP evaporator. Any steam level other than the LP needs at least three heat exchangers: one for the economiser (where subcooled water is heated close to its saturation point), one for the evaporator and one for the superheating of steam. One or more HR units can be considered for the economiser and for superheating according to the design practice of HRSG (Stecco et al., 1991), (Gator-Power, 1994), but their arrangement is a difficult optimisation problem that will be solved through a synthesis model.

The fundamentals for the derivation of a network superstructure from (Floudas et al., 1986), (Floudas and Ciric, 1989), (Biegler et al., 1997a) were applied to the HRSG synthesis problem and the resulting rules are:

1. Split the gas turbine exhaust stream through as many as potential heat recovery (HR) exchangers as may exist.
   There will be one HR for LP steam generation and at least 3 (economiser, evaporator and superheater) for any other steam pressure level. Manufactures of HRSG may use up to three heat recovery coils for economisers and for superheaters (Gator-Power, 1994), (Dechamps, 1998) and only one HR exchanger for the evaporation section.

2. From the outlet of each HR exchanger split the gas turbine exhaust to the other match inlets and to the target mixer for the stream.

3. Apply a similar procedure to the cold side (i.e. water/steam streams), but the splitting/mixing will depend on the particular HR type of sections (i.e. economisers or evaporators or superheaters).

By following the above synthesis procedure, a superstructure that contains all stream interconnections among the heat recovery equipments in a HRSG is obtained. This contains all configurations with and without stream splitting, with mixing and with possible bypass streams. The optimal stream interconnections as well as the number and position of HR exchangers are
determined from the solution of a synthesis MINLP model.

The proposed superstructure may have a very large number of variables because it involves no decomposition such as is sometimes used in heat exchanger network synthesis. Decomposition implies the sequential calculation of minimum utilities and units as well as heat loads for the calculated heat exchangers using LP and MILP, see (Floudas et al., 1986).

The search space however is bounded using logical constraints for defining for instance that a superheater (SH) needs an evaporator (EV) and this needs the existence of an economiser (EC). The whole MINLP model for a double pressure steam system is given in Section 3.5.4.

A hyperstructure involves several superstructures and contains all the possible alternatives in a synthesis problem (Floudas and Ciric, 1989). The hyperstructure for the synthesis of HR coils in HRSG contains a superstructure for the hot side streams and a superstructure for the cold side streams.

The next subsection shows a double pressure steam system as an example for the hyperstructure derivation for the optimal synthesis of HR coils in a HRSG. Based on this example it will be easy to develop a general hyperstructure to consider all the possible arrangements of HR exchangers for steam generation according to current HRSG design practice see (Gator-Power, 1994), (Stecco et al., 1991) and (Dechamps, 1998) and even some other arrangements possibly not explored by commercial designers of HRSG.

3.5.3 Hyperstructure for the synthesis of HR exchangers in the HRSG of a double pressure steam system

The concepts for defining a hyperstructure (Floudas and Ciric, 1989) were adapted for CHP systems. Following the basic principles for superstructure derivation the hyperstructure for a HRSG producing steam at two pressure levels was proposed and represented by the superstructure for the hot side streams, Fig. 3.4, and by the superstructure for the cold side streams, Fig. 3.5. Note that in both superstructure diagrams the HR exchangers are represented, but they do not have duplicated performance.

A double pressure steam HRSG considers the generation of low pressure (LP) and high pressure (HP) steam. The HRSG consists of 8 possible heat recovery (HR) sections (see Fig. 3.5):
Now, we propose the:

**Hyperstructure model for a double pressure steam system**

Consider a hyperstructure having $N_{HR}$ heat recovery exchangers. For a double pressure steam system $N_{HR} = 8$ (see Fig. 3.4 and Fig. 3.5). The following units have to be modelled,

a) For defining the HRSG hyperstructure:

1. LP evaporator with steam drum

![Diagram of Hyperstructure model for a double pressure steam system](image)

Figure 3.4: Hot side superstructure for HRSG synthesis. Here only three potential heat recovery exchangers are shown.
Figure 3.5: Cold side superstructure for HRSG synthesis. Example for a double pressure steam system.
2. three potential HP economisers
3. HP evaporator with steam drum
4. three potential HP superheaters.

b) Hot streams superstructure (gas turbine exhaust side):

1. split the gas turbine exhaust into $N_{HR}$ streams
2. $N_{HR}$ mixers with $N_{HR}$ input streams and a single output stream
3. $N_{HR}$ splitters with $N_{HR}$ output streams and a single input stream
4. the gas turbine exhaust is collected in a mixer target having $N_{HR}$ input and 1 output streams

c) Cold streams superstructure (water/steam side):

1. split HP subcooled water in as many streams as potential HP economisers $N_{HP EC}$ may exist (in this case $N_{HP EC} = 3$)
2. $N_{HP EC}$ mixers with $N_{HP EC}$ input streams and a single output stream
3. $N_{HP EC}$ splitters with $N_{HP EC}$ output streams and a single input stream
4. HP water is collected in a mixer (at the target point) having $N_{HP EC}$ input and 1 output streams. This mixer then sends preheated water (near its saturation point) to the HP steam drum, see mixer 'MCS 4' in Fig. 3.5
5. split HP saturated steam from HP steam drum in as many streams as potential HP superheaters $N_{HP SH}$ may exist (in this case $N_{HP SH} = 3$)
6. $N_{HP SH}$ mixers with $N_{HP SH}$ input streams and a single output stream
7. $N_{HP SH}$ splitters with $N_{HP SH}$ output streams and a single input stream
8. HP superheated steam is collected in a mixer (at the target point) having $N_{HP SH}$ input and 1 output streams. This mixer then sends superheated steam to steam turbines or to external users, depending of the CHP system.
3.5.4 MINLP model for HR exchangers synthesis in HRSG

Following the double pressure steam system example, mentioned in the last subsection, the MINLP model consists of minimising the O.F. given by equation (3.31) subject to:

1. Splitter models
   For gas turbine exhaust and water/steam sides defining the hyperstructure.

2. Mixer models
   For gas turbine exhaust and water/steam sides defining the hyperstructure.

3. Equipment Models
   A CHP system having steam turbines, air-cooled condenser, steam drums, gas turbine, pumps, deaerator, etc.

4. Integer variables
   Integer variables 'z' have potential values of (0 or 1). An integer variable $z_{i, HR}$ is proposed for every HR exchanger (8 for the double pressure steam example, see Fig. 3.5):
   - $z_{LP \ EV}$ = integer variable associated with the existence of the LP evaporator
   - $z_{HP \ EC_i}$ = integer variable associated with the existence of up to 3 HP economisers ($i = 1, 2, 3$)
   - $z_{HP \ EV}$ = integer variable associated with the existence of the HP evaporator
   - $z_{HP \ SH_i}$ = integer variable associated with the existence of up to 3 HP superheaters ($i = 1, 2, 3$)

5. Logical constraints for connecting the heat loads to the integer variables
   The HR exchangers are described by the EO model given in Appendix D, Section D.3 for continuous optimisation problems and by such model with the additional next constraints for MINLP synthesis problems,
   \[ Q_i - Q_i^U z_i \leq 0 \quad (3.32) \]
   where $(i = 1, \ldots, N_{HR})$
   For FMS, the modelling language used (described in Chapter 5), we need slack variables to transform this and any other inequality constraint into an equality constraint. e.g. in this case,
   \[ Q_i - Q_i^U z_i + s_i = 0 \quad (3.33) \]
Note that every logical constraint transformed into an equality uses its own slack variable $s_i$.

6. Logical constraints for connecting the heat transfer area of HR exchangers to the integer variables

$$A_i - A^U_i z_i \leq 0$$  \hspace{1cm} (3.34)

7. Equations for relating the cold and hot side ('cs' and 'hs' respectively) stream flowrates to the integer variable of each HR, \(i = 1, \ldots, N_{HR}\)

$$F_{cs_i} - F_{cs}^U z_i \leq 0$$  \hspace{1cm} (3.35)

$$F_{hs_i} - F_{hs}^U z_i \leq 0$$  \hspace{1cm} (3.36)

8. Logical constraints for the temperature range through HR exchangers

The temperature range (change in temperature of a given stream when passing through a heat exchanger) is related to integer variables by the equations given below.

The temperature range for the cold stream,

$$T_{csr_i} = T_{co} - T_{ci}$$  \hspace{1cm} (3.37)

needs a logical constraint given by,

$$T_{csr_i} - T_{cs}^U z_i \leq 0$$  \hspace{1cm} (3.38)

while for the hot stream the temperature range,

$$T_{hsr_i} = T_{hi} - T_{ho}$$  \hspace{1cm} (3.39)

needs a logical constraint given by,

$$T_{hsr_i} - T_{hs}^U z_i \leq 0$$  \hspace{1cm} (3.40)

9. Constraints relating integer variables to pressure drop through HR exchangers

The nonexistence of a HR exchanger \((z = 0)\) required the addition of the condition that the pressure drops $\Delta P_{cs}$, $\Delta P_{hs}$ for cold and hot side respectively should be zero for \(z = 0\).

In the synthesis strategy of this research pressure drops for a HR exchanger are treated as specifications. They are denoted by $\Delta P_{fcs}$ and $\Delta P_{fhs}$ for cold and hot side respectively.

Thus, the following constraints relating pressure drops to integer variables were proposed,
Cold side

\[ \Delta P_{fe} \cdot z_i = \Delta P_{cs} \]

(3.41)

where,

\[ \Delta P_{cs} = P_{1, cs} - P_{2, cs} \]

Hot side

\[ \Delta P_{fs} \cdot z_i = \Delta P_{hs} \]

(3.42)

\[ \Delta P_{hs} = P_{1, hs} - P_{2, hs} \]

(3.43)

Additional modelling equations for binary variables including propositional logical expressions (Floudas, 1995), (Biegler et al., 1997a) were adapted for this HRSG synthesis model. This are given below,

10. From the three HP economisers, select at least one unit

\[ z_{HP \ EC1} + z_{HP \ EC2} + z_{HP \ EC3} \geq 1 \]

(3.44)

11. From the three HP superheaters, select at least one unit

\[ z_{HP \ SH1} + z_{HP \ SH2} + z_{HP \ SH3} \geq 1 \]

(3.45)

12. For the statement "If any of the HP superheaters (SH) is selected, then the HP evaporator (EV) must be selected"

The corresponding equivalent logical constraint is derived below.

Consider the following logical operators,

<table>
<thead>
<tr>
<th>Logical operator</th>
<th>symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>.OR.</td>
<td>\lor</td>
</tr>
<tr>
<td>.AND.</td>
<td>\land</td>
</tr>
<tr>
<td>.NOT.</td>
<td>\neg</td>
</tr>
</tbody>
</table>

Such statement is an implication that may be written as,

\[ (z_{HP \ SH1} \lor z_{HP \ SH2} \lor z_{HP \ SH3}) \implies z_{EV} \]

(3.46)

(a) replace the implication by its equivalent disjunction,

generically if \( P_1 \) are a set of clauses:

\[ P_1 \implies P_2 \iff \neg P_1 \lor P_2 \]
or,
\[ \neg \left( z_{HP \ SH1} \lor z_{HP \ SH2} \lor z_{HP \ SH3} \right) \lor z_{EV} \]

(b) Apply DeMorgan's Theorem (Floudas, 1995) to put the negation inward, generically:

\[ \neg (P_1 \lor P_2) \iff \neg P_1 \land \neg P_2 \]

we have,

\[ \left( \neg z_{HP \ SH1} \land \neg z_{HP \ SH2} \land \neg z_{HP \ SH3} \right) \lor z_{EV} \]

(c) Distribute the logical operator \( \lor \) over the logical operator \( \land \) recursively, using:

\[ (P_1 \land P_2) \lor P_3 \iff (P_1 \lor P_3) \land (P_2 \lor P_3) \]

so we have,

\[ \left( \neg z_{HP \ SH1} \lor z_{EV} \right) \land \left( \neg z_{HP \ SH2} \lor z_{EV} \right) \land \left( \neg z_{HP \ SH3} \lor z_{EV} \right) \]

Thus, the original statement "If any of the superheaters (SH) is selected, then the evaporator (EV) must be selected" is equivalently written in mathematical form as the next independent constraints,

\[ z_{HP \ SH1} - z_{HP \ EV} \leq 0 \quad (3.47) \]
\[ z_{HP \ SH2} - z_{HP \ EV} \leq 0 \quad (3.48) \]
\[ z_{HP \ SH3} - z_{HP \ EV} \leq 0 \quad (3.49) \]

13. For the statement "If any of the HP Economisers (EC) is selected, then the HP evaporator (EV) must be selected",

as in the last set of constraints we have now,

\[ z_{HP \ EC1} - z_{HP \ EV} \leq 0 \quad (3.50) \]
\[ z_{HP \ EC2} - z_{HP \ EV} \leq 0 \quad (3.51) \]
\[ z_{HP \ EC3} - z_{HP \ EV} \leq 0 \quad (3.52) \]

14. For the statement "If evaporator (EV) is selected then at least one of the HP economisers (HP EC) must be selected" we have,

\[ 1 - z_{EV} + z_{HP \ EC1} + z_{HP \ EC2} + z_{HP \ EC3} \geq 1 \]

or,

\[ z_{EV} - (z_{HP \ EC1} + z_{HP \ EC2} + z_{HP \ EC3}) \leq 0 \quad (3.53) \]
15. **Logical constraint for the statement** "If evaporator (EV) is selected then at least one of the HP superheaters (HP SH) must be selected".

This constraint ensures the generation of HP superheated steam, which is required in our CHP systems,

\[ z_{EV} - (z_{HP SH1} + z_{HP SH2} + z_{HP SH3}) \leq 0 \]  

(3.54)
Chapter 4

Mathematical software packages

This chapter describes the mathematical techniques implemented in the packages used for EO simulation, optimisation and synthesis.

Since we proposed a complete EO model for CHP systems, we needed to demonstrate its applicability. This was evaluated by solving from small to large-scale complex simulation problems. One of them was a cogeneration plant in operation whose simulation, using the proposed model, reproduced very well the performance of the real plant (see Chapter 6, Section 6.6.4).

For the solution of complex simulation problems in a simultaneous approach we need: (a) to have a square system without redundant equations nor free variables, and (b) to supply a starting guess for the solution of the system of equations by a Newton-type method.

In our new EO environment (described in Chapter 5) we use an Equation Analyser (Morton and Collingwood, 1998) to identify redundant equations and free variables (see Section 4.1.1.) and a sparse Nonlinear Algebraic Equations solver (Morton, 1997) aimed at improving the robustness of Newton's method (Section 4.1.2).

Even though the mathematical methods used for NLP optimisation (Section 4.2) and for synthesis (Section 4.3) are designed to provide global convergence (i.e. from any starting point) we found that their efficient performance needed the supply of a warm starting guess, obtained by simulation. This is because of the complex nature of CHP systems.
4.1 Packages for EO simulation

4.1.1 The equation analyser (EA)

The EA (Morton and Collingwood, 1998) is intended to help the engineer to deal with some of the problems encountered in process modelling (Westerberg and Benjamin, 1985). It can:

- perform structural analysis of a system of equations, detecting redundant equations and free or unspecified variables;
- perform a numerical check on the equations (using sparse Gaussian Elimination (Chen and Stadtherr, 1984)) so as to detect singular linear or nonlinear subsets of equations.

Since the EA can find the redundant equations and free variables in a model, it can be used to identify variables to be associated with the degrees of freedom. This is especially important prior to performing an EO simulation.

4.1.2 Sparse nonlinear algebraic equations (NLAE) solver

For solving the simultaneous equations defining a simulation problem we used a new sparse nonlinear algebraic equations (NLAEs) solver. This code, described elsewhere (Morton, 1997), has a number of features aimed at improving robustness compared with the straightforward application of Newton's method when the starting guess is far from the solution, while preserving the second-order rate of convergence close to the solution. However, no single panacea guarantees complete robustness. The solver's features include the following:

- A **singular equation solver** (SES) can find a partial solution of singular, sparse linear equations. We can therefore use without concern about initial guesses for NLAEs which generate a singular linearisation.

- **"Hard" bounds on variables** are used to prevent unphysical values (e.g. negative compositions) or mathematical function errors (e.g. logarithm of a negative number) and may also be used to keep the solution estimate within a physically expected range (by imposing reasonable upper bounds, for example, on flows, temperatures and heat duties).
In addition to variable bounds, a trust region (TR) may be used, to restrict the step at each Newton iteration. The TR is a square region around the current solution estimate within which the next step must lie. Its size may increase or decrease as the NLAEs solution proceeds, depending on how closely the previous Newton linearisation approaches the NLAEs surface over the step just taken. The TR is applied to scaled variables. Scaling refers to the use of scale factors for each equation and variable and is applied consistently to derivatives (see Chapter 5, Section 5.5).

A step restriction procedure is needed in the case that the solution of the Newton linearisation lies outside the TR or variable bounds. Three methods are compared in (Morton, 1997). In all the runs reported in Chapter 6, any variable which crosses a variable bound or TR bound is restricted to lie on the bound after the step. This method ("variable chopping") has generally been found to work well.

In the runs described in Chapter 6, norm reduction for the equation residuals is not enforced and the sparse linearised equations are reordered to limit fill-in using the SPK1 method (Stadtherr and Wood, 1984a).

Convergence of the NLAEs normally requires reducing both the maximum error ($L_\infty$ norm of the scaled nonlinear equation residuals) and the maximum step size ($L_\infty$ norm of the scaled step size) below user-adjustable tolerances.

If the solution becomes trapped by bounds and the step size remains below the tolerance while the equations are unconverged for more than 5 iterations then the simulation is ended with a 'solution stalled' indication. The simulation also may end at a user-supplied maximum iteration count.

### 4.2 Packages for SQP optimisation

Successive Quadratic Programming (SQP) has proved to be an efficient and robust method for nonlinear programming problems, and is suitable for large-scale problems (Biegler, 1992). SQP has the advantage (over for instance, Generalised Reduced Gradient methods) of not requiring convergence of the equality constraints at intermediate points. In addition, since it is a Newton-based method, SQP has quadratic convergence properties, and generally requires few function evaluations. Nevertheless, when the size of the problem becomes large, the cost of the optimisation is dominated by the Newton (QP) step. A SQP strategy is less sensitive to a
poor initial guess than other codes like MINOS, an implementation of an augmented projected Lagrangian algorithm (Vasantharajan et al., 1990).

The basic SQP method solves a sequence of QP problems where the objective function is expressed in a quadratic approximation in the form of the Hessian of the Lagrangian. The solution of each quadratic programming (QP) problem provides a step 's' towards the new point.

The results obtained at the optimised solution satisfy the Kuhn-Tucker conditions (which summarise the first and second order optimality conditions) and the code will find: the optimised objective function; the full set of variables x that gives the optimal solution; and the Lagrange multipliers, which are weakly positive for active lower bounds, weakly negative for active upper bounds and zero for the inactive constraints. The reduced Hessian of the Lagrangian in the null space of active constraints (equations and active bounds) should be positive definite for a constrained local minimum.

To obtain the solution of the NLP problem satisfying the 1st and 2nd order optimality conditions, the system model is solved simultaneously with the optimisation problem. A few more details are given below.

The SQP method can be referred as a Lagrange-Newton method (Fletcher, 1987) since it can be explained in terms of Newton's method applied to find the stationary point of the Lagrangian function \( L \) given by,

\[
L = f(x) - \sum_k \lambda_k c_k
\]

where \( c_k \) is the set of constraints, \( f(x) \) is the objective function and \( \lambda_k \) are the Lagrange multipliers.

A feature of the SQP methods is the generation of a sequence of \( x \) and \( \lambda \) which approximate the solution vector \( x^* \) and the optimal \( \lambda^* \).

Consider the application of Newton's method to the first order Kuhn-Tucker (KT) conditions (Fletcher, 1987) to get the Newton equations in SQP (equations 4.1-4.4):

\[
\sum_j \frac{\partial^2 L}{\partial x_i \partial x_j} s_j - \sum_k \frac{\partial c_k}{\partial x_i} \Delta \lambda_k - \sum_p \frac{\partial g_p}{\partial x_i} \Delta u_p = -\frac{\partial L}{\partial x_i} \tag{4.1}
\]

\[
\sum_j \frac{\partial c_k}{\partial x_j} s_j = -c_k \tag{4.2}
\]
\[
\sum_j \frac{\partial g_{ip}}{\partial x_j} s_j = -g_{ip} \quad (4.3)
\]
\[
\Delta u_{ip} = -u_{ip} \quad (4.4)
\]

where \( s \) is the proposed step in \( x \), \( u_p \) are the Lagrange multipliers for the inequality constraints \( g_p \). Subscripts \( A \) and \( I \) refer to active and inactive constraints respectively. In this case the Newton's method gives corrections to \( x \) and Lagrange multipliers.

The Newton's equations constitute the KT conditions for the sequence of QP problems. The quadratic objective function \( L_Q \) in the QP problem has linearised constraints. So the QP problems are given by,

\[
\begin{align*}
\min L_Q &= L_0 + s^T \nabla L + \frac{1}{2} s^T H s \\
\text{subject to:} & \\
& c_0 + s^T \nabla c = 0 \\
& g_0 + s^T \nabla g \geq 0
\end{align*} \quad (4.5)
\]

where Hessian of the Lagrangian, \( H \), and gradient of Lagrangian, \( \nabla L \), are evaluated at the starting guess for the iteration.

During the iterations in a SQP method a sequence of QP problems which approximate the NLP is done. In addition a line search is calculated to ensure descent direction for a penalty function (which tries to decrease the objective and constraint violations).

During the iterative procedure the first order KT conditions are checked for convergence, the QP is solved and the line search obtained. In addition the second order KT conditions,

\[
v^T \nabla^2 L v > 0 \quad (4.6)
\]

are verified for all feasible directions \( v \).

Other SQP methods can use a trust region (TR) rather than a line search to restrict the step (Fletcher, 1987). A constraint containing the TR is added to the constraints in the QP problem (equation 4.5). For a given step \( \Delta x \) the method changes the TR value depending on how well the QP approximates the original problem. The use of exact Hessian (obtained by the explicit calculation of partial derivatives) needs a strategy (e.g. a trust region) to ensure a bounded QP when the Hessian is non-positive definite.

The early stages of this research involved the use of a SQP method which employs a 'tolerance-tube' approach (Zoppke-Donaldson, 1995) to decide whether to accept a step from the QP
subproblem. Later we use a Modelling Package, FMS (described in Chapter 5, Section 5.1) and the filterSQP solver (Fletcher and Leyffer, 1998), an advanced method with a ‘filter’ to promote global convergence. Both optimisation codes are described below.

4.2.1 ‘Tolerance-Tube’ SQP method

This code has a recent implementation of the SQP method (Zoppke-Donaldson, 1995), which uses a ‘tolerance tube’ to decide whether or not each step solved by a QP point approximation of the NLP is acceptable. In common with older SQP methods a succession of QP problems is solved, each with quadratic objective and linear constraints which are a pointwise local approximation to the NLP problem. However, the ‘Tolerance-Tube’ method does not need a penalty parameter to weight constraint violations relative to the objective.

A quasi-Newton Hessian approximation is dense and is unsuitable for large problems, so a sparse version is used here. Furthermore, by using the exact Hessian we should obtain true second order convergence near the solution, rather than superlinear convergence.

The main characteristics of this SQP solver are (Zoppke-Donaldson, 1995):

- it uses a novel strategy to restrict the step in the QP problem, by insisting that the step remains inside a “tolerance-tube”, defined by a maximum sum of constraint violations;
- a second-order correction step (SOC) (Fletcher, 1987) is taken if the QP step moves outside the ‘tolerance-tube’;
- where a QP is infeasible a “Phase I” LP is solved to minimise the sum of linearised constraint violations in the QP;
- a trust region approach is used to increase or decrease the maximum step size according to how well the QP just solved approximates the NLP locally. Steps which violate the ‘tolerance-tube’ even after second order correction are rejected and cause a reduction of the trust region.

The tolerance-tube restriction replaces the traditional insistence on doing an inexact line search in some penalty function which weights constraint violations and the objective, using a suitably large but essentially arbitrary penalty parameter for the constraints.
4.2.2 ‘FilterSQP’ method

A new SQP trust region algorithm has been developed at the University of Dundee (Fletcher and Leyffer, 1998) following on from the ‘Tolerance-Tube’ SQP method. This method is known as ‘filterSQP’. It also avoids using a penalty parameter to weight the constraints and objective, and contains a number of improvements.

The NLP algorithm uses a SQP with the called ‘filter-type method’ to promote global convergence. The method has several heuristics aiming to eliminate situations where the solver might fail (e.g. the need to unblock ‘filter’ in some situations), see (Fletcher and Leyffer, 1997).

The main features of filterSQP method are (Fletcher and Leyffer, 1998):

- A SQP trust region algorithm is used with a convergence strategy called a “filter” aimed to promote global convergence. The “filter” is a list of pairs of objective function values and norm of constraint violations;
- A new step is accepted whenever it improves the objective or the constraints compared to the filter: if not the step is rejected;
- As in the case of the ‘Tolerance-Tube’ SQP method the trust region size is changed adaptively by the algorithm, and if a step is rejected the trust region is reduced;
- The algorithm terminates when it has found a Kuhn-Tucker point or no further progress appears to be possible;
- Each iteration is characterised by the success of the step taken; by the SQP solver phase (i.e. feasibility iteration or normal SQP); by the order of the step (Linear Programming, QP, second order correction or unblocked); and, where applicable by any heuristics applied as explained in (Fletcher and Leyffer, 1997).
- Dense and sparse filterSQP versions are available.

4.3 Synthesis code

For the synthesis problems we propose a MINLP model (see Chapter 3, Section 3.5) that was solved with the MINLP_BB package (Leyffer, 1998). This package solves MINLP problems.
by branch and bound using a depth-first-search. These problems are given by NLP problems containing some variables which can take only integer values.

4.3.1 ‘MINLPBB’ package

The MINLP_BB package has a branch and bound strategy for the integer part of the problem and the filterSQP method (described in Section 4.2.2 for the continuous optimisation part. (Leyffer, 1998) reports that this solver is more robust than Outer Approximation (Duran and Grossmann, 1986) or generalised Benders decomposition, see e.g. (Floudas, 1995).

The branch and bound solver uses a sparse strategy to solve efficiently problems with many integer variables. In the branch and bound method the search is done in a branch and bound tree. The MINLP_BB solver has improved techniques for the identification of lower bounds (Leyffer, 1998) that can reduce the number of NLP problems that need to be solved in the tree search. The method includes a branching rule that uses the lower bounds to decide on the next fractional variable to branch. It also possesses the capability for the user to influence the branching decision. This is done by giving priorities for the integer variables, so the solver would branch on the variable with the highest priority first. When no priorities are given, the variable with the most distant (from the lower bound) fractional value is selected for branching.

4.3.2 Branch and bound scheme

A branch and bound scheme is used to solve problems having both integer and continuous variables. This is a general method for solving problems with integer variables in a combinatorial space. The optimal integer values are determined by a tree search in which relaxations of the mixed-integer problem (with integer variables considered as continuous) are solved and non-integer relaxation solutions are eliminated by adding simple bounds, namely by branching.

A branch and bound tree has nodes with branches to potential values of integer variables (1 or 0). To limit the tree search and avoid complete enumeration, lower and upper bounds on the optimal objective value are used.

Consider a MINLP problem $P_{mi}$ with an objective function $(O.F.)$, mixed constraints with variables $x$ having $x_j$ integer variables $j \in I$, and a set $X$ representing simple bounds on variables. Consider that the feasible region is bounded. Let $P'_{mi}$ be the problem obtained
from \( P_{mi} \) by relaxing integer variables.

Problem \( P'_{mi} \) is a normal NLP problem. In the first step of a branch and bound method \( P'_{mi} \) is solved with a solution \( x' \). If \( x' \) involves feasible values for all the integer variables then it is an integer feasible. Since the integer feasible also is a solution to \( P_{mi} \) then the algorithm finishes. If the algorithm does not finish in the first step, then there exists at least one variable \( x_j^f \), \( j \in I \) which is fractional. The scheme then branches on a relaxed integer variable with fractional value, e.g. \( x_j^f \), and introduces two different subproblems coming from \( P_{mi} \) by adding the simple constraints \( x_j = 1 \) and \( x_j = 0 \) to each subproblem respectively. The optimal solution to problem \( P_{mi} \) is contained in the feasible region of one of the two added subproblems, and the branching procedure can be rerun.

The branch and bound algorithm then solves more subproblems in a tree search. Nodes in a tree refer to NLP problems. A fathomed node describes a fully explored node. In this algorithm entire subtrees can be eliminated from explicit evaluation after their root node has been fathomed. Fathomed nodes are those identified as infeasible or those producing an integer feasible solution. The last-mentioned case provides an upper bound to the optimal value of problem \( P_{mi} \). Such an upper bound serves to prune nodes with optimal value (or lower bound) greater than or equal to the current upper bound.

### 4.3.3 A small example showing the branching scheme in MINLP_BB

This simple example shows how the branch and bound scheme for MINLP problems works. The example is taken from (Duran and Grossmann, 1986) and was solved to evaluate the MINLP_BB/FMS interface (Chapter 5, Section 5.4) before attempting the large synthesis problems (Chapter 8). A description of the problem is,

\[
\begin{align*}
\min_{x,z} & \quad 5z_1 + 6z_2 + 8z_3 + 10x_1 - 7x_3 - 18 \ln(x_2 + 1) \\
& \quad -19.2 \ln(x_1 - x_2 + 1) + 10 \\
\text{subject to} & \quad 0.8 \ln(x_2 + 1) + 0.96 \ln(x_1 - x_2 + 1) - 0.8x_3 \geq 0 \\
& \quad \ln(x_2 + 1) + 1.2 \ln(x_1 - x_2 + 1) - x_3 - 2z_3 \geq -2 \\
& \quad x_2 - x_1 \leq 0 \\
& \quad x_2 - 2z_1 \leq 0 \\
& \quad x_1 - x_2 - 2z_2 \leq 0 \\
& \quad z_1 + z_2 \leq 1 \\
& \quad 0 \leq x \leq u, \text{ where } u^T = (2, 2, 1) \\
& \quad 0 \leq z_i \leq 1
\end{align*}
\]

We use a value of zero for all variables in the starting guess and no branching priority on integer variables was given.
Branching iterations

Using the MINLP_BB package, the branch and bound sequence in the tree search was obtained and is represented in Fig. 4.1. The tree search is as follows,

A problem 0 got a not integer feasible solution with $O.F. = 0.759$ (at the top of Fig. 4.1).

The algorithm then branches on $z_2 = 0.3$ (being the highest relaxed integer variable in this NLP since $z^T = (0.2732, 0.3, 0.0)$).  \(^1\)

The method then introduces 2 new problems: problem 1 with $z_2 = 0$ and problem 2 with $z_2 = 1$.

B problem 1 is solved to a not integer feasible solution with $O.F. = 5.1713$. Branch on $z_1 = 0.5$ (the highest from $z = (0.5, 0.0, 0.0)$).

Introduce 2 new problems: problem 3 with $z_1 = 0$ and problem 4 with $z_1 = 1$.

C problem 3 is the next solved (after problem 1, see also Fig. 4.1) due to the fact that the algorithm has a depth-first-search of the tree. Here it found an integer feasible which is a new upper bound with $O.F. = 10.000$ and $z^T = (0.0, 0.0, 0.0)$. At this point we have two problems remaining on stack (i.e. problem 2, and problem 4 in Fig. 4.1). Since the algorithm has the additional feature that backtracking is done to the most promising node then the new top problem is the number 2 with $O.F$ estimate 0.759.

D problem 2 then converged the NLP with $O.F. = 6.0098$ and $z^T = (0.0, 1.0, 0.0)$ to an integer feasible which is a new upper bound. Thus the number of problems remaining on stack is 1 (i.e. problem 4).

E problem 4 got a NLP solution with $O.F. = 7.0927$. This solution is dominated by upper bound, therefore we fathom this node (implying the non-necessity for branching on $z_3$).

The MINLP_BB solver finished the solution of this problem.

A summary of the results from the MINLP_BB solver for this small test problem is reported in Table 4.1. It should be mentioned that, since this test problem is convex, then we found the global optimum.

\(^1\) The values for the continuous variables are not given in this tree search description since they are not directly relevant to the branching procedure.
Figure 4.1: Duran-Grossmann problem showing MINLP.BB branching iterations.

Table 4.1: Solution to Duran and Grossmann MINLP problem.

<table>
<thead>
<tr>
<th>Results from MINLP.BB solver</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>0.35</td>
</tr>
<tr>
<td>Number of NLPs solved:</td>
<td>5</td>
</tr>
<tr>
<td>Number of NLPs generated:</td>
<td>5</td>
</tr>
<tr>
<td>Total number of QPs solved:</td>
<td>22</td>
</tr>
<tr>
<td>... of which infeasible QPs:</td>
<td>0</td>
</tr>
<tr>
<td>Average number of QPs solved per NLP:</td>
<td>4.4</td>
</tr>
<tr>
<td>Average CPU time for NLPs (s):</td>
<td>0.07</td>
</tr>
<tr>
<td>Function evaluations</td>
<td>22</td>
</tr>
<tr>
<td>Constraint evaluation</td>
<td>27</td>
</tr>
<tr>
<td>Gradient evaluations</td>
<td>27</td>
</tr>
<tr>
<td>Final value f(x*)</td>
<td>6.00975</td>
</tr>
<tr>
<td>x* (continuous variables)</td>
<td>(1.301, 0.0, 1.0)</td>
</tr>
<tr>
<td>z* (integer variables)</td>
<td>(0.0, 1.0, 0.0)</td>
</tr>
</tbody>
</table>
Chapter 5

Equation oriented modelling framework

The solution of large-scale problems in a simultaneous approach embraces, in addition to the use of efficient solvers and careful modelling of individual units, the creation of large models (putting together many individual units) represented in a huge data structure. The large-scale models then should interact with mathematical solvers for a number of applications.

The core of our EO framework for modelling, simulation, optimisation and synthesis is the *Flexible Modelling System*, FMS (Mitchell and Morton, 1996) a program developed under our research group. FMS is a generic equation-based modelling package to build and solve problems in an EO approach.

With FMS we can set up large systems of equations, create networks to be modelled, give starting guesses and scale factors easily for problems of any size. Also FMS is able to interact with our solvers, described in Chapter 4, for EO simulation, optimisation and synthesis.

This chapter begins with an explanation of the Modelling System as well as some examples on models created using FMS. Then we include a brief description of how models in FMS interact with solvers and details of the filterSQP/FMS and the MINLP_BB/FMS interfaces. Scaling for the former and the implementation of an interface to the latter were added to the original FMS program by the author of this thesis. Finally, this chapter has a description of the scaling procedure for variables, constraints and derivative information as well as a list of FMS commands used in this work.
It should be mentioned that in this chapter FMS is described only in terms of its capabilities used for modelling CHP systems. We do not give a complete description of the many features and capacities of the modelling system, which is fully described in (Mitchell, 1999).

### 5.1 Flexible Modelling System, FMS

In order to specify general process engineering problems, a new modelling language for EO simulation, optimisation and synthesis, known as the Flexible Modelling System (FMS), has been developed. This system is described in more detail elsewhere (Mitchell and Morton, 1996). In FMS we can easily set up large systems of simultaneous equations defining a model. The original FMS version made available for this research had interfaced a set solvers for use in EO simulation (as described in Chapter 4, Section 4.1) and an early version of the filterSQP optimisation code which did not include scaling.

For the solution of NLP optimisation and synthesis problems new sparse solvers needed to be interfaced to FMS for use in this research. FMS allows us rapidly to construct interfaces to stand-alone solvers such as the optimisation software from R. Fletcher's group at The University of Dundee, U.K. for NLP and MINLP problems, described in Chapter 4 (Sections 4.2.2 and 4.3.1 respectively).

Other desirable attributes of FMS include:

- the ability to set up large systems of modelling equations;
- the facility to create models for large networks containing individual unit models, or models of sub-sections of plants and to build complex models from simpler ones as in ASCEND (Piela et al., 1991). For instance, a plant section can be modelled by properly interconnecting the relevant streams and unit operations models. Several plant sections can then be linked to model a whole plant;
- an easy way to initialise the variables in a flowsheet and to give variable and equation scale factors. Starting guesses are easily given including 'warm starts' which are converged solutions to sub-models;
- the ability to call different codes of solution including:
  - an Equation Analyser (EA) (Morton and Collingwood, 1998) to check models for correct specification and find block structure;
- a sparse Non-linear Algebraic Equations (NLAЕ) Solver (Morton, 1997) which was used for the EO simulation examples in Chapter 6;
- a new SQP code named "filterSQP" (Fletcher and Leyffer, 1998) used in the Non-linear Optimisation problems shown in Chapter 7;
- a new code for solving MINLP problems with a branch and bound scheme, named "MINLP_BB" (Leyffer, 1998) used for the synthesis problems presented in Chapter 8;
- a Genetic Algorithm (GA) which is currently under investigation (but not applied in this research) to allow automatic starting guess generation.

- routines in which modelling equations and partial derivative information are coded, for use by the above solvers;
- the capability to set fixed specifications in a given model. These are the fixed values which constrain to the model's degrees of freedom.
- FMS displays a variable list including bounds, and has the capability to show the equation list, residuals list, the Jacobian matrix $J$, $\frac{\partial f_o}{\partial x}$ and Hessian matrix $H$, obtained from the second partial derivatives $\frac{\partial^2 f_o}{\partial x_i \partial x_j}$ and $\frac{\partial^2 f_o}{\partial x_i \partial x_j}$. All of those lists and matrices can be seen before and after the application of a mathematical code for solving a given problem.

A description of the data format to create models and how some models were built in FMS is detailed below.

5.1.1 How to build a model in FMS

For modelling CHP systems in this research, we have to provide FMS with all the streams and unit operations models (mentioned in Chapter 3, Sections 3.1 - 3.2 and in Appendices A - D). The proposed modelling equations, the 1st partial derivatives and the 2nd partial derivatives of every constraint type with respect to each variable were programmed by the author of this thesis in Fortran 90 for FMS usage.

Having defined individual models we further used FMS to construct models for process streams, complex units (like gas turbines), sub-sections of plants and whole utility systems. To actually construct a model we needed to fill in standard data formats about individual models and about

\[ f_o \] represents any modelling equation.
variable information which the Modelling Language is able to use. To fully explain this, a few introductory definitions are given below.

1. **Entity type (ETYPE).** This is basically an individual model which may be re-used for constructing larger models or networks, e.g.: process streams, unit operations, a set of interconnected unit operations defining sub-sections of plants, etc. Entity types (models) are defined by filling in a basic data format in FMS (see Fig. 5.1) containing information about variables, equations, stream inter-connections of unit operations, etc. Some characteristics of the 'entity types' are,
   - they can use previously defined models (or entity types);
   - they may contain variables and equations defined by the user;
   - the user may interconnect streams to/from unit operation models (etypes previously defined) to model networks;
   - the user may supply a starting guess to override variables-default values;
   - the user may fix some variables, e.g. to some (or all) of the *degrees of freedom* for a given model;
   - the user may supply variable scale factors to ignore default values;
   - user supplied numerical values should be given as real values.

   Information about the model is defined in FMS by using the *keywords* as detailed below.

2. **Keywords for the basic format for defining 'entity types' in FMS.** To define a model we need to fill in a basic data format in FMS. In the FMS version used here the basic format is actually created in a computer editor (e.g. XEmacs) and involves a general structure that uses *keywords*, some of them being optional, depending of the kind of model defined. *Keywords* are presented in capital letters in the FMS format representation in Fig. 5.1. A short description for them is shown in Table 5.1. These *keywords* are reserved for FMS usage and should not be given to name e.g. variables, equations, or models.

3. **Variable type (VTYPE).** This is the user supplied information required to designate default bounds, value and scale factor for variables of certain ‘type’ e.g. temperature, mass flow, mole fraction, etc. (see Chapter 3, Sections 3.1 - 3.2 and Appendices A - D for details on all the proposed modelling variables and equations). A ‘variable type’ for every generic variable should be declared by the user in a data file created with a computer editor. Details on the *keywords* used to define a generic ‘variable type’ are given in Table 5.2.
CHAPTER 5. EQUATION ORIENTED MODELLING FRAMEWORK

Figure 5.1: Basic format in FMS to define an entity type (a model).

<table>
<thead>
<tr>
<th>FMS keyword</th>
<th>User supplied information</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETYPE</td>
<td>model (or entity type) name.</td>
</tr>
<tr>
<td>VARS</td>
<td>declare variables used by the model giving name and 'variable type' (VTYPE). For vectors give size as well.</td>
</tr>
<tr>
<td>INSTANCE</td>
<td>declare previously defined models (ETYPEs) to be used in current ETYPE.</td>
</tr>
<tr>
<td>EQNS</td>
<td>declare an equation giving the name of the Fortran 90 subroutine where it is defined and a list of variables that the equation needs.</td>
</tr>
<tr>
<td>CONNECT</td>
<td>to declare that two models are equivalent and their variables and equations should not be declared twice (e.g. an OUT-stream of a unit being the IN-stream of another).</td>
</tr>
<tr>
<td>FIXED</td>
<td>to declare fixed variables in the model.</td>
</tr>
<tr>
<td>ASSIGN</td>
<td>to change default starting guesses, bounds and scale factors.</td>
</tr>
<tr>
<td>END</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.1: Keywords used to define 'entity types' (models) in FMS.
Table 5.2: *Keywords* used to define 'variable types' in FMS.

<table>
<thead>
<tr>
<th>FMS keyword</th>
<th>User supplied information</th>
</tr>
</thead>
<tbody>
<tr>
<td>VTYPE</td>
<td>variable type name</td>
</tr>
<tr>
<td>UBOUND</td>
<td>variable upper bound</td>
</tr>
<tr>
<td>LBOUND</td>
<td>variable lower bound</td>
</tr>
<tr>
<td>VALUE</td>
<td>variable default value (to initialise problems)</td>
</tr>
<tr>
<td>SCALE</td>
<td>variable scale factor (if not supplied, FMS considers 1.0)</td>
</tr>
<tr>
<td>END</td>
<td></td>
</tr>
</tbody>
</table>

5.1.2 Specifying modelling equations in FMS

In this research, general equations \( c(x) \) (constraints in optimisation problems) were given in Fortran 90 routines\(^2\) in the form required by FMS,

\[ c(x) = 0 \]

where the left hand side evaluation, being non-zero before the equation has been satisfied, is known as 'the residual'.

Suppose we want to model in FMS an equation having two variables. In the 'entity type' data format along with the *keyword* EQNS (see Table 5.1) we should indicate information about the equation as shown in Table 5.3. In this table 'entity type name' denotes the identification of the model in which 'variable.1' (and 'variable.2') were defined. If 'variable.1' is actually firstly defined in the current model we use a dot '. '. Note that a semicolon ';' is added after all variables used in the equation are specified (see also Fig. 5.1). This concepts will be clearly understood by looking at the example of a simulation model constructed in FMS (see the next subsection).

5.1.3 Examples of simulation models in FMS

A simple example for a valve is shown to illustrate how simulation models were built in FMS.

\(^2\) Fortran 90 routines contain the equation, 1st and 2nd partial derivative information in an appropriate way which FMS can process.
Table 5.3: Defining an equation in FMS.

<table>
<thead>
<tr>
<th>EQNS</th>
<th>user supplied equation name</th>
</tr>
</thead>
<tbody>
<tr>
<td>entity type name variable_1 name</td>
<td>entity type name variable_2 name</td>
</tr>
<tr>
<td>;</td>
<td></td>
</tr>
</tbody>
</table>

**FMS model for a valve**

Consider the EO model for a valve (detailed in Section D.14, Appendix D) where air is the kind of stream in consideration. This example consists in preparing data to define a model in FMS. A valve is illustrated as follows,

![Diagram of a valve](image)

To model a valve, we need an EO mathematical model for:

- IN-stream,
- OUT-stream,
- the valve itself.

Let's see the process stream model first. Consider an air stream with a single pseudocomponent (whose model was detailed in Chapter 3, Section 3.1.2). The model for this stream contains 7 variables:

- \( F, P, h, H, T, s, v \).
These variables are respectively: mass flow, pressure, specific enthalpy, enthalpy flow, temperature, specific entropy and specific volume.

We proposed 4 equations to define this stream type:

\[ H - h_F = 0 \quad (5.1) \]
\[ h - h_a(T, P) = 0 \quad (5.2) \]
\[ s - s_a(T, P) = 0 \quad (5.3) \]
\[ v - v_a(T, P) = 0 \quad (5.4) \]

where the subscript 'a' refers to air thermodynamic properties. So we have 7 variables and 4 equations for a single air stream.

The corresponding 'entity type' (model definition) in FMS for an air stream with a single pseudocomponent is given in Table 5.4. This was taken directly from our actual data file defining 'entity types'. Note that for a given 'entity type' (depending on the specific model) we do not need to use all the keywords described earlier in Table 5.1. What is very important in the definition of equations is that the list of variables in the data format (in Table 5.4) should follow the same order as the one given in the Fortran 90 routine defining the equation. This is because this order is used in FMS to construct the model list of variables.

The specification of two intensive variables, like \( P, T \) (or \( h \)) and one extensive variable, like \( F \), allows the simultaneous solution of the above 4 nonlinear equations to describe fully an air process stream. Note that the ETYP for air stream in Table 5.4 is a generic air stream model that may be used to model streams in unit operations or to simulate a simple air stream. To do the later one has to create another ETYP 'calling' the ETYP for air stream and fixing the mentioned 3 degrees of freedom.

For our simple example of the valve model we have defined in FMS the process streams. Now as mentioned in Appendix D, Section D.14 the valve model is given by,

\[ F_2 - F_1 = 0 \quad (5.5) \]
\[ H_2 - H_1 = 0 \quad (5.6) \]
\[ P_2 - P_1 + \Delta P = 0 \quad (5.7) \]

The ETYP for the valve is shown in Table 5.5. Again, this ETYP for a valve is a generic model that may be used in a network or stand alone.

Note that the valve model expressed for FMS in Table 5.5 has one degree of freedom for this
unit (i.e. the valve $\Delta P$, according to Appendix D, Section D.14) and also three degrees of freedom for the IN-stream (i.e. $P$, $T$ or $h$ and $F$). Suppose we want to simulate an air stream with $F = 10\ kg/s$, $T = 400\ ^\circ C$ and $P = 0.5\ MPa$ passing through a valve whose pressure

Table 5.4: ‘Entity type’ (model definition) for air streams in FMS.

<table>
<thead>
<tr>
<th>ETYPE</th>
<th>Air_Str_Single_Comp</th>
</tr>
</thead>
<tbody>
<tr>
<td>VARS</td>
<td></td>
</tr>
<tr>
<td>FF</td>
<td>mass_flow</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
</tr>
<tr>
<td>h_for_FMS</td>
<td>specific_enthalpy</td>
</tr>
<tr>
<td>HH</td>
<td>enthalpy_flow</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
</tr>
<tr>
<td>s</td>
<td>entropy</td>
</tr>
<tr>
<td>v</td>
<td>gas_sp_v</td>
</tr>
<tr>
<td>EQNS</td>
<td></td>
</tr>
</tbody>
</table>

```
ETYPE       Air_Str_Single_Comp
VARS
FF          mass_flow
P           pressure
h_for_FMS   specific_enthalpy
HH          enthalpy_flow
T           temperature
s           entropy
v           gas_sp_v
EQNS
H_flow
  . h_for_FMS
  . FF
  . HH
;
Air_Single_Comp_Str_enthalpy
  . h_for_FMS
  . T
  . P
;
Air_Single_Comp_Str_entropy
  . s
  . T
  . P
;
Air_Sp_V
  . v
  . T
  . P
;
END
```
drop is $\Delta P = 0.2\, MPa$. The ETYPE modelling the EO simulation of such a valve is given in Table 5.6. Note in such table how the specification of fixed variables is actually expressed. With this ETYPE FMS sets up the simulation model having 11 equations and 15 variables, but the specification of 4 of them gave a square system of equations.

Table 5.5: 'Entity type' for a valve in FMS.

<table>
<thead>
<tr>
<th>ETYPE</th>
<th>Valve</th>
</tr>
</thead>
<tbody>
<tr>
<td>VARS</td>
<td>deltaP: pressure_drop</td>
</tr>
<tr>
<td>INSTANCE</td>
<td>Air_Str_Single_Comp</td>
</tr>
<tr>
<td></td>
<td>IN_stream</td>
</tr>
<tr>
<td></td>
<td>OUT_stream</td>
</tr>
<tr>
<td>EQNS</td>
<td>Material_Balance</td>
</tr>
<tr>
<td></td>
<td>IN_stream: FF</td>
</tr>
<tr>
<td></td>
<td>OUT_stream: FF</td>
</tr>
<tr>
<td></td>
<td>Valve_Energy_Balance</td>
</tr>
<tr>
<td></td>
<td>IN_stream: HH</td>
</tr>
<tr>
<td></td>
<td>OUT_stream: HH</td>
</tr>
<tr>
<td></td>
<td>Momentum_Balance</td>
</tr>
<tr>
<td></td>
<td>IN_stream: P</td>
</tr>
<tr>
<td></td>
<td>OUT_stream: P, deltaP</td>
</tr>
<tr>
<td></td>
<td>END</td>
</tr>
</tbody>
</table>
CHAPTER 5. EQUATION ORIENTED MODELLING FRAMEWORK

5.1.4 List of variables produced by FMS

To further explain a few capabilities of FMS, let us continue with the simple simulation model for a valve for which the corresponding ETYPE was given in Table 5.6.

When we actually run FMS we set up our valve simulation model by typing the ETYPE named 'Valve_simul' (see Table 5.6). The model is created by FMS and then we typed the command 'dv' to see a full list of variables. Note that variables for IN/OUT streams as well as local (unit) variables are clearly identified by FMS (see Table 5.7).

The list of variables in FMS include (see Table 5.7):

- 'Var no.', which is the variable number;
- 'Entity' identification (e.g. Valve_simul.V_1);
- 'Variable' name;
- 'Value';
- 'L_Bnd', which is the lower bound for each variable;
- 'U_Bnd', which is the upper bound;

Table 5.6: 'Entity type' for the simulation of a valve with air streams in FMS.

<table>
<thead>
<tr>
<th>ETYPE</th>
<th>Valve_simul</th>
</tr>
</thead>
</table>

| INSTANCE
<table>
<thead>
<tr>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Valve</td>
</tr>
<tr>
<td>V_1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>FIXED</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>V_1.IN_stream FF value 10.0</td>
<td></td>
</tr>
<tr>
<td>V_1.IN_stream P value 0.5</td>
<td></td>
</tr>
<tr>
<td>V_1.IN_stream T value 400.0</td>
<td></td>
</tr>
<tr>
<td>V_1 deltaP value 0.2</td>
<td></td>
</tr>
</tbody>
</table>

END
Table 5.7: Set up a model and variable list from FMS for an air stream through a valve (showing fixed (Stat=1) and default (Stat=0) values).

FMS: Build model from type : Valve_simul

FMS:: d v

Variables: pattern * : *

<table>
<thead>
<tr>
<th>Var no.</th>
<th>Entity</th>
<th>Variable</th>
<th>Value</th>
<th>L_Bnd</th>
<th>U_bnd</th>
<th>Stat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Valve_simul.V_1</td>
<td>deltaP</td>
<td>200.000E-03</td>
<td>0.000E+00</td>
<td>14.000E+00</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>FF</td>
<td>10.000E+00</td>
<td>0.000E+00</td>
<td>31.000E+00</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>P</td>
<td>500.000E-03</td>
<td>1.000E-03</td>
<td>14.000E+00</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>h_for_FMS</td>
<td>2.500E+03</td>
<td>1.000E+00</td>
<td>5.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>HH</td>
<td>85.000E+03</td>
<td>0.000E+00</td>
<td>50.000E+06</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>T</td>
<td>400.000E+00</td>
<td>10.000E-03</td>
<td>6.000E+03</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>s</td>
<td>50.000E+00</td>
<td>10.000E-03</td>
<td>100.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>Valve_simul.V_1.IN_stream</td>
<td>v</td>
<td>100.000E-06</td>
<td>90.000E-06</td>
<td>300.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>FF</td>
<td>1.000E+00</td>
<td>0.000E+00</td>
<td>31.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>P</td>
<td>1.500E+00</td>
<td>1.000E-03</td>
<td>14.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>h_for_FMS</td>
<td>2.500E+03</td>
<td>1.000E+00</td>
<td>5.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>HH</td>
<td>85.000E+03</td>
<td>0.000E+00</td>
<td>50.000E+06</td>
<td>0</td>
</tr>
<tr>
<td>13</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>T</td>
<td>300.000E+00</td>
<td>10.000E-03</td>
<td>6.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>14</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>s</td>
<td>50.000E+00</td>
<td>10.000E-03</td>
<td>100.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>Valve_simul.V_1.OUT_stream</td>
<td>v</td>
<td>100.000E-06</td>
<td>90.000E-06</td>
<td>300.000E+00</td>
<td>0</td>
</tr>
</tbody>
</table>
5.1.5 Examples of optimisation models in FMS

To explain how an optimisation model was constructed using FMS, consider the general form of a NLP optimisation problem (as described in Chapter 3, Section 3.4),

\[
\begin{align*}
\min & \quad O.F. = f(x) \\
\text{subject to:} & \quad c_i(x) = 0.0 \\
& \quad x_L < x < x_U
\end{align*}
\]

(5.8)

there, the constraint equations \( c_i(x) \) and the bounds on variables \( x_L, x_U \) can properly be defined using FMS in ETYPES and VTYPEs (as explained in Sections 5.1.1 and 5.1.2). For modelling optimisation problems we could have a simple ETYPE containing all the constraint functions (say ETYPE 1). Then for constructing the optimisation model in FMS, we define a new ETYPE (say ETYPE 2) which uses the ETYPE 1 and has only one modelling equation (the objective function, O.F.). One can also define O.F. and constraints in a single ETYPE (practical only for small problems). The only condition is that, when defining ETYPES for optimisation problems in FMS, the first equation should be the objective function.

A first example on how we construct an optimisation model in FMS considers a combined cycle power plant consisting of:

- a gas turbine (GT)
- a heat recovery steam generator (HRSG)
- 2 steam turbines
- condensing equipment, pumps and valves

the problem was to optimise the plant’s thermal efficiency,

\[
\eta_{th} = \frac{\Sigma W_i}{Q}
\]

(5.9)

where \( W_i \) is the gas and steam turbines power output and \( Q \) is the heat given to the CHP plant (to the gas turbine combustor).
When modelling this plant in FMS we constructed ETYPES first for basic entities (e.g. process streams, individual unit operations) then we linked together all the required ETYPES to construct a single ETYPE involving all the modelling equations (constraints). Such a single ETYPE was called 'GT_hrsg_2turb_link' and was used in the ETYPE modelling this optimisation problem (see Table 5.8). In this table, note that the ETYPE 'C_2t_0pt' declares only one equation, which is the objective function 'O.F. Gen_Therm_Eff'. This objective function uses variables for the number of turbines 'No_turb', the O.F. scale factor, heat load and power from turbines (see Table 5.8). Comments in an ETYPE are added after typing '#'.

The second example for ETYPE of an optimisation problem considers the MINLP problem presented in Chapter 4, Section 4.3.3 (Duran and Grossmann, 1986). The ETYPE for the MINLP model is presented in Table 5.9. This ETYPE (named 'Duran_Grosm_Op_MINLP') has only one modelling equation, i.e. the objective function 'Objective'. The constraints for the problem were actually declared in a separate ETYPE (not shown here) named 'Duran_Grosm_MINLP'. Note also in Table 5.9 how the starting guess is given for continuous and integer variables 'x_i' and 'z_i' respectively, and how using an asterisk '*' we refer to all elements in a vector for slack variables 'slack.*'.

Note that a single optimisation model in FMS (represented in an ETYPE) may be defined by including the objective function followed by all the constraints. However, we constructed a separate ETYPE for the constraints which in turn was used by an 'optimisation' ETYPE that declares the objective function as the only equation. In this way we could use individual models (e.g. for a gas turbine) in as many models as we wanted.

5.2 Models interacting with solvers in FMS

By summing up the concepts given in Section 5.1 we could say that a complete model in FMS can be represented as in the upper part of in Fig. 5.2 and comprises:

- modelling equations, 1st and 2nd partial derivatives (programmed in Fortran 90 and linked to FMS);
- entity types, ETYPES (as defined in subsection 5.1.1);
- variable types, VTYPES (as defined in subsection 5.1.1);

3 Note that NLP and MINLP problems can be modelled in similar way in FMS, since both have an objective function and a set of constraints.
Table 5.8: 'Entity type' in FMS for a combined cycle power plant.

<table>
<thead>
<tr>
<th>ETYPE</th>
<th>C_2t_Opt</th>
</tr>
</thead>
<tbody>
<tr>
<td>VARS</td>
<td></td>
</tr>
<tr>
<td>ObF_scal</td>
<td>size</td>
</tr>
<tr>
<td>No_turb</td>
<td>size</td>
</tr>
<tr>
<td>INSTANCE</td>
<td></td>
</tr>
<tr>
<td>GT_HRSG_2turb_linked</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>EQNS</td>
<td></td>
</tr>
<tr>
<td>Gen_Term_Eff</td>
<td></td>
</tr>
<tr>
<td>c.gt.Burn</td>
<td>Qf</td>
</tr>
<tr>
<td>c.gt</td>
<td>Wout</td>
</tr>
<tr>
<td>c.P.Turb_1</td>
<td>W</td>
</tr>
<tr>
<td>c.P.Turb_2</td>
<td>W</td>
</tr>
<tr>
<td>FIXED</td>
<td></td>
</tr>
<tr>
<td>.</td>
<td>ObF_scal</td>
</tr>
<tr>
<td>.</td>
<td>No_turb</td>
</tr>
<tr>
<td>ASSIGN</td>
<td></td>
</tr>
<tr>
<td>*</td>
<td>deltaP</td>
</tr>
<tr>
<td>### a 'warm' starting guess follows in original ETYPE</td>
<td></td>
</tr>
<tr>
<td>### (in a data file), but was not included here</td>
<td></td>
</tr>
</tbody>
</table>

Definition of a given model then requires its solution. For the problems solved in this research we could choose simulation, optimisation or synthesis packages (described in Chapter 4). FMS has now interfaced these mathematical codes as shown in Fig. 5.2. Scaling on filterSQP/FMS interface and the implementation of MINLP_BB/FMS interface were a contribution from this research. Both interfaces are briefly explained in the next subsections.
Table 5.9: ‘Entity type’ in FMS for a MINLP problem (Duran and Grossmann, 1986).

<table>
<thead>
<tr>
<th>VARS</th>
<th>ObF_scal</th>
<th>size</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>INSTANCE</th>
<th>Duran_Grosm_MINLP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>One</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EQNS</th>
<th>Objectiv</th>
</tr>
</thead>
<tbody>
<tr>
<td>One</td>
<td>nvar</td>
</tr>
<tr>
<td>One</td>
<td>x_var_1</td>
</tr>
<tr>
<td>One</td>
<td>x_var_2</td>
</tr>
<tr>
<td>One</td>
<td>x_var_3</td>
</tr>
<tr>
<td>One</td>
<td>z_i_1</td>
</tr>
<tr>
<td>One</td>
<td>z_i_2</td>
</tr>
<tr>
<td>One</td>
<td>z_i_3</td>
</tr>
<tr>
<td>ObF_scal</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>FIXED</th>
<th>One nvar value 6.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>One</td>
<td>ObF_scal value 1.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ASSIGN</th>
<th>One x_var_1 value 0.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>One</td>
<td>x_var_2 value 0.0</td>
</tr>
<tr>
<td>One</td>
<td>x_var_3 value 0.0</td>
</tr>
<tr>
<td>One</td>
<td>z_i_1 value 0.0</td>
</tr>
<tr>
<td>One</td>
<td>z_i_2 value 0.0</td>
</tr>
<tr>
<td>One</td>
<td>z_i_3 value 0.0</td>
</tr>
<tr>
<td>One</td>
<td>slack.* value 1.0</td>
</tr>
</tbody>
</table>

5.3 FilterSQP/FMS interface

The interface between FMS and the NLP optimisation package filterSQP is represented in Fig. 5.3. With this interface we pass a fully scaled problem to filterSQP while objective function,
CHAPTER 5. EQUATION ORIENTED MODELLING FRAMEWORK

Figure 5.2: A complete model and solvers interfaced to FMS.
This interface has two Fortran 90 programs (see Fig. 5.3):

1. ‘Driver program’.

That gets the required parameters from FMS to call the main routine from filterSQP (as described in (Fletcher and Leyffer, 1998)). The ‘driver program’ also scales starting guess variables and bounds on variables and gets the following user supplied information:

- printing option from filterSQP;
- the ‘output channel’ (6 for screen);
- optimisation problem name;
- the expected minimum value for the objective function;
- trust region value;
- solver tolerance;
- maximum number of iterations.

Figure 5.3: Schematic representation for the filterSQP/FMS interface.
2. ‘NLP information transfer program’.

That allows filterSQP to work with a fully scaled problem while constraints \(c_i(x)\), objective function \(f\), Jacobian matrix \(J\) and Hessian matrix \(H\) are calculated unscaled in their calculation routines.

### 5.4 MINLP\_BB/FMS interface

This interface consists only of a driver program. This is because the MINLP\_BB solver used the filterSQP method whose interface was described in last section.

In this case, the driver program calls the main routine for the MINLP\_BB solver (Leyffer, 1998) and scales variables and bounds on variables. These are then passed to the MINLP\_BB solver. At running time, this driver program gets from the user:

- MINLP solver tolerance;
- printing option;
- the ‘output channel’ (6 for screen);
- the choice to print (or not) the SQP iterations;
- the choice to print (or not) information from the QP problems;
- MINLP problem name;
- priorities for branching on integer variables (optional);
- trust region value;

### 5.5 Scaling procedure

In a typical utility system optimisation problem the variables like heat loads, temperatures, enthalpies, entropies, steam quality, mole fraction, etc. are all of very different orders of magnitude. As mentioned in (Fletcher and Leyffer, 1998) the filterSQP solver could be inefficient in these circumstances where the trust region does not discriminate between variables of different magnitudes. A scaling procedure was then implemented and is described below:
1. The strategy followed for scaling the problems was to present the optimiser a fully scaled problem, i.e. to scale (and unscale) variables, constraints, bounds and derivative information in an interface between the SQP solver and the calculation subroutines. Thus the solver optimised a fully scaled problem while the model calculation subroutines worked with an unscaled problem. This interface interacts with FMS and was described in Section 5.3

2. Variables were scaled by dividing them by their typical value in integer powers of ten. The scaled variables are then of the same order of magnitude (about unity). For instance for a gas turbine combustor, the OUT-stream has \( T = 1265^\circ C \) and the scale factor is \( 1.0 \times 10^3 \). For the variables \( x_j \) we introduce scale factors \( w_j \), so the scaled variables \( \xi_j \) of order 1, are given by:

\[
\xi_j = x_j / w_j \quad (5.10)
\]

This scaling procedure was also used to scale variable lower and upper bounds.

3. Constraints \( c \) were scaled by dividing them by the typical value of a given term or group of terms in integer powers of ten, e.g. for the constraint,

\[ h \ F - H = 0 \]

the constraint scale factor may be \( 1.0 \times 10^4 \) (the scale factor for the \( H \) variable for a given stream in kW). In this case we define constraint scale factors \( t_i \) to get the scaled constraints \( \gamma_i \) from:

\[
\gamma_i = c_i / t_i \quad (5.11)
\]

4. For the objective function \( f \) we use an objective scale factor \( u \) so the scaled objective \( \varphi \) is,

\[
\varphi = f / u \quad (5.12)
\]

5. The 1st partial derivative information of a given constraint was scaled dividing by the corresponding constraint scale and multiplying by the relevant variable scale factor, or:

\[
\frac{\partial \gamma_i}{\partial \xi_j} = \left( \frac{w_j}{t_i} \right) \frac{\partial c_i}{\partial x_j} \quad \text{or} \quad (5.13)
\]

6. The 2nd partial derivative information of a given constraint with respect to variables \( x_j, x_k \) was scaled multiplying by the scale factors of both variables in the Hessian element and dividing by the equation scale factor, or:

\[
\frac{\partial^2 \gamma_i}{\partial \xi_j \partial \xi_k} = \left( \frac{w_j w_k}{t_i} \right) \frac{\partial^2 c_i}{\partial x_j \partial x_k} \quad (5.14)
\]
This scaling method for partial derivatives was also applied to the objective function and its partial derivatives.

7. Since the filterSQP worked with a fully scaled problem, then at solution we unscale variables, constraints, bounds on variables, objective function, and Lagrange multipliers. To explain how unscaled multipliers are obtained, recall that in FMS we express an optimisation problem in the form:

\[
\begin{align*}
\min & \quad O.F. = f(x) \\
\text{subject to} & \quad c_i(x) = 0.0 \\
& \quad x_L < x < x_U
\end{align*}
\]

So we use slack variables to convert inequality into equality constraints. The Kuhn-Tucker (KT) conditions (Fletcher, 1987) require:

\[
\begin{align*}
\nabla f - (\nabla c)^T \lambda - (\mu_L - \mu_U) &= 0 \quad (5.15) \\
c(x) &= 0 \quad (5.16)
\end{align*}
\]

where \( \lambda \) are multipliers for the equations and \( \mu_L, \mu_U \) are the multipliers for variable lower and upper bounds.

The Newton step (Fletcher, 1987) involves the solution of:

\[
\begin{align*}
Gs - A\lambda - (\mu_L - \mu_U) &= -\nabla f_0 \quad (5.17) \\
A^T s &= -c_0 \quad (5.18)
\end{align*}
\]

where \( 's' \) is the step in \( 'x' \), \( G \) is the Hessian of the Lagrangian:

\[
G_{ij} = \frac{\partial^2 L}{\partial x_i \partial x_j} \quad (5.19)
\]

and \( A \) is the transpose of the constraints Jacobian:

\[
A_{ij} = \frac{\partial c_i}{\partial x_j} \quad (5.20)
\]

We know that \( \mu = 0 \) for inactive variable bounds (being determined by the NLP optimiser). Thus, we can define the Lagrangian function \( L \) (unscaled) as,

\[
L = f - c^T \lambda - (x - x_L)^T \mu_L - (x_U - x)^T \mu_U \quad (5.21)
\]

therefore,

\[
G_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j} - \sum_k \frac{\partial^2 c_k}{\partial x_i \partial x_j} \lambda_k \quad (5.22)
\]
In order to express a scaled Newton step (from equation 5.17), we introduce diagonal scaling matrices $W$, $T$ for variable and constraint scale factors: $W_{jj} = w_j$ and $T_{ii} = t_i$.

Then if $\sigma$ is the scaled step, of order 1, and $\Lambda$ is the scaled Lagrangian:

\begin{align*}
  s & = W \sigma \\
  x & = W \xi \\
  c & = T \gamma \\
  f & = u \varphi \\
  \nabla f & = u W^{-1} \nabla \xi \varphi \\
  \nabla L & = u W^{-1} \nabla \xi \Lambda \\
  G & = u W^{-1} \nabla^2 \xi \Lambda W^{-1} \\
 & = u W^{-1} \Gamma W^{-1} \\
 A & = \nabla c^T = W^{-1} \nabla \xi \gamma^T T \\
 & = W^{-1} \mathcal{K} T
\end{align*}

where $\Gamma$ is the scaled Hessian and $\mathcal{K}$ is the scaled Jacobian transpose. $\nabla \xi$ denotes partial derivatives with respect to the scaled variables $\xi$. The scaled stationary condition (from equation 5.17) for the Newton step becomes:

\begin{equation}
(u W^{-1} \Gamma W^{-1}) (W \sigma) - W^{-1} \mathcal{K} T \lambda - (\mu_L - \mu_U) = -u W^{-1} \nabla \xi \varphi_0
\end{equation}

or, multiplying by $W/u$,

\begin{equation}
\Gamma \sigma - (1/u) \mathcal{K} T \lambda - (W/u)(\mu_L - \mu_U) = -\nabla \xi \varphi_0
\end{equation}

From last equation, the scaled multipliers $\beta$ and $\theta_L, \theta_U$ for equations and variable bounds must be given by:

\begin{align*}
  \beta_i & = (t_i/u) \lambda_i \\
  \theta_{Lj} & = (w_j/u) \mu_{Lj} \\
  \theta_{Uj} & = (w_j/u) \mu_{Uj}
\end{align*}

Thus, from the above equations we can unscale the Lagrange multipliers (obtained from the scaled problem) after the final solution from the filterSQP code has been obtained.
5.6 Commands used in FMS

A list of FMS commands (Mitchell and Morton, 1996) used in this research is presented in Table 5.10.

Table 5.10: FMS commands used in this research.

<table>
<thead>
<tr>
<th>FMS command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>d v</td>
<td>displays all variables</td>
</tr>
<tr>
<td>d f</td>
<td>displays fixed variables</td>
</tr>
<tr>
<td>i</td>
<td>initialise variable values (to starting guess)</td>
</tr>
<tr>
<td>ea</td>
<td>executes the Equation Analyser</td>
</tr>
<tr>
<td>s solver</td>
<td>followed by a solver's identification</td>
</tr>
<tr>
<td></td>
<td>this command sets the solver from:</td>
</tr>
<tr>
<td></td>
<td>- bil.nlae</td>
</tr>
<tr>
<td></td>
<td>- filter</td>
</tr>
<tr>
<td></td>
<td>- MINLP_BB</td>
</tr>
<tr>
<td>e</td>
<td>executes the selected solver</td>
</tr>
<tr>
<td>d e</td>
<td>displays equations</td>
</tr>
<tr>
<td>d r</td>
<td>displays constraints' residuals</td>
</tr>
<tr>
<td>d j</td>
<td>displays Jacobian</td>
</tr>
<tr>
<td>d h</td>
<td>displays Hessian</td>
</tr>
</tbody>
</table>
Chapter 6

Simulation results and discussion

This chapter reports a number of simulation problems for combined heat and power (CHP) systems solved by simultaneous equations. The range of problems cover from individual streams and units up to and including complete utility systems. For each problem we provide a brief description, results given by the number of iterations (from the sparse NLAE solver, described in Chapter 4, Section 4.1.2) and their analysis. The problem descriptions contain: physical characteristics; data on the size of simulation models (including the number of variables, the number of equations and the number of degrees of freedom \(^1\)); and a description of the specifications, or fixed variable values, that must be given for each degree of freedom in the initial model. Then at the end of this chapter we present an analysis of the performance of the equation oriented (EO) packages and of the proposed EO models used for simulation.

The models for each problem were constructed in FMS, using equation based models written in Fortran 90 for individual equipment and process streams in utility systems (detailed in Chapter 3, Sections 3.1 - 3.2 and Appendices A - D). These models supply equation residuals and partial derivative information to solvers as required.

Except where stated, a default initial guess is defined in FMS for each type of variable and used to start the solution. Default initial guesses are defined in FMS by using variable types (VTYPES), as explained in Chapter 5, Section 5.1.1.

\(^1\) equal in number to the difference between variables and equations.
6.1 How do we solve EO simulation problems

For a given EO model we count the number of variables and equations to get the number of degrees of freedom. In the early stages of the research this was done by 'manual inspection' producing tables for equations and variables in models. Later, for large-scale problems, we took data on number of variables and equations directly from FMS (e.g. for the model in Section 6.5.5).

In general, fixing degrees of freedom in our simulation models was proposed by properly selecting independent stream variables and unit parameters (Westerberg et al., 1979). Once a given model was defined in FMS (as explained in Chapter 5, Sections 5.1.1 - 5.1.3), we then checked that our specifications made sense for the independent set of modelling equations to be solved.

Each model was run through the equation analyser EA (described in Chapter 4, Section 4.1.1) to check the formulation, identifying redundant equations and free variables (see Fig. 6.1). After the model has been checked and the EA detects no modelling errors and no free variables the simulation problems were then solved. Note however that some complex models (e.g. where a hyperstructure was included) have many recycles to mixers which make some of the momentum balance equations redundant (Section 6.5.5), but still the simulations could be done successfully.
For complex simulation problems (e.g. several units linked) "warm-start" initial guesses were used by overwriting the default guesses with converged values from separately solved subsystems. This can be done easily within FMS. Warm guesses were used for problems in Sections 6.4 - 6.6.

The general procedure applied to solve simulation models is explained by describing a simple example. Consider a water/steam stream (model described in Chapter 3 Section 3.1.1) where we fixed $F$, $T$ and $q = 0$ to specify a saturated vapour stream. Its simulation model was defined and then set up with FMS (see Table 6.1). Then we run the EA typing 'ea', and we do not use a control file (meaning that the EA uses default parameters (Morton and Collingwood, 1998)). The successful identification of zero redundant equations and zero free variables was then followed by running the NLAE solver. To do this we set the solver (using FMS command 's'), see Table 6.2, and execute the solver (using FMS command 'e') with default parameters (including no use of a trust region (TR) (Morton, 1997)). After convergence, we display the resulting variable values (using FMS command 'd v'), see Table 6.2.

Default starting guess for general water/steam streams is given by the values in Table 6.1. This was used in all the simulation problems in this chapter, except otherwise specified in individual models.

We start presenting EO simulation problems for individual process streams and unit operations (Sections 6.2 and 6.3). We then present examples which build up from elementary units to the simulation of complex unit operations and plant sections (Sections 6.4 and 6.5). Among the complex unit operations units, a full commercial gas turbine simulation (including the compression, fuel/air mixing, combustion and turbine sections) is given in Section 6.4.1. A heat recovery steam generator (HRSG) with three pressure levels is simulated in Section 6.4.2, where separate components at different pressures are dealt with in HRSG-subsections. In Section 6.4.3 the complete HRSG is drawn together. Section 6.5.2 combines the gas turbine and HRSG, while a water/steam distribution system is simulated in Section 6.5.3.

Thanks to the capabilities of FMS, by linking plant sections' models we could easily build up complete utility systems models (Section 6.6). Warm-start guesses were used to simulate successfully large-scale problems (with up to about 3,000 variables).

It should be mentioned that water/steam and air (single pseudo-component) streams models

---

2 In Table 6.1 we show the variables for this model: $F$ [kg/s], $P$ [MPa], $h$, $h_f$, $h_g$ [kJ/kg], $H_H$ [kW], $T$, $T_s$ [$^\circ$C], $s$ [kJ/kg K], $\phi$, $q$ [-] and specific volume 'sp.vol' [m$^3$/kg].
Table 6.1: Set up a water/steam model and variable list from FMS (showing fixed (Stat=1) and default (Stat=0) values) and EA run.

<table>
<thead>
<tr>
<th>Var no.</th>
<th>Entity</th>
<th>Variable</th>
<th>Value</th>
<th>L_Bnd</th>
<th>U_bnd</th>
<th>Stat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>New_Wat_St_Str</td>
<td>FF</td>
<td>1.00E+00</td>
<td>0.00E+00</td>
<td>2.00E+00</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>New_Wat_St_Str</td>
<td>P</td>
<td>1.50E+00</td>
<td>1.00E-06</td>
<td>1.25E+00</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>New_Wat_St_Str</td>
<td>h</td>
<td>2.50E+03</td>
<td>1.00E+00</td>
<td>5.00E+03</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>New_Wat_St_Str</td>
<td>HH</td>
<td>8.50E+03</td>
<td>0.00E+00</td>
<td>5.00E+06</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>New_Wat_St_Str</td>
<td>T</td>
<td>1.00E+00</td>
<td>1.00E-03</td>
<td>6.00E+03</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>New_Wat_St_Str</td>
<td>s</td>
<td>5.00E+00</td>
<td>1.00E+00</td>
<td>1.00E+00</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>New_Wat_St_Str</td>
<td>phi</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>1.00E+00</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>New_Wat_St_Str</td>
<td>q</td>
<td>0.00E+00</td>
<td>-1.00E+00</td>
<td>1.00E+00</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>New_Wat_St_Str</td>
<td>Ts</td>
<td>3.00E+00</td>
<td>1.00E+00</td>
<td>3.50E+03</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>New_Wat_St_Str</td>
<td>hf</td>
<td>1.00E+03</td>
<td>1.00E+00</td>
<td>2.00E+03</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>New_Wat_St_Str</td>
<td>hg</td>
<td>3.50E+03</td>
<td>2.00E+03</td>
<td>5.00E+03</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>New_Wat_St_Str</td>
<td>sp_vol</td>
<td>1.00E-03</td>
<td>9.00E-06</td>
<td>3.00E+00</td>
<td>0</td>
</tr>
</tbody>
</table>

FMS:: Build flowsheet using entity type : New_Wat_St_Str

FMS:: d v

Give name of output file *.nlae: temporary

Is there an EqAnalyser control file? (y/n, default n) n

Completed output assignment : 0 redundant eqns
                                0 free variables.

Matrix blocking performed

Completed Gauss elimination : 0 redundant eqns
                              0 free variables.

Equation system analysed. All done.
Table 6.2: Running NLAIE solver (only two iterations shown) and simulation results for a water/steam model from FMS.

FMS:: s solver bill_nlae
FMS:: e

Is there an EqSolver control file? (y/n, default n)
n
Solution history

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Maximum scaled error</th>
<th>reord eqn</th>
<th>1 = equation</th>
<th>Maximum scaled step</th>
<th>in reord var</th>
<th>2 = variable</th>
<th>2 = variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>60000.</td>
<td>1</td>
<td>H_flow</td>
<td>94.949</td>
<td>2</td>
<td>P</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Maximum scaled error</th>
<th>reord eqn</th>
<th>2 = equation</th>
<th>Maximum scaled step</th>
<th>in reord var</th>
<th>12 = variable</th>
<th>12 = variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.65938E-10</td>
<td>2</td>
<td>Wat_Seam_h</td>
<td>0.32318E-11</td>
<td>12</td>
<td>sp_vol</td>
<td></td>
</tr>
</tbody>
</table>

FMS:: d v

<table>
<thead>
<tr>
<th>Var no.</th>
<th>Entity</th>
<th>Variable</th>
<th>Value</th>
<th>L_Bnd</th>
<th>U_Bnd</th>
<th>Stat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>New_Wat_St_Str</td>
<td>FF</td>
<td>10.000E+00</td>
<td>0.000E+00</td>
<td>20.000E+00</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>New_Wat_St_Str</td>
<td>P</td>
<td>101.396E-03</td>
<td>100.000E-06</td>
<td>12.500E+00</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>New_Wat_St_Str</td>
<td>h</td>
<td>2.676E+03</td>
<td>1.000E+00</td>
<td>5.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>New_Wat_St_Str</td>
<td>HH</td>
<td>26.761E+03</td>
<td>0.000E+00</td>
<td>50.000E+06</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>New_Wat_St_Str</td>
<td>T</td>
<td>100.000E+00</td>
<td>10.000E-03</td>
<td>6.000E+03</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>New_Wat_St_Str</td>
<td>s</td>
<td>7.350E+00</td>
<td>10.000E-03</td>
<td>100.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>New_Wat_St_Str</td>
<td>phi</td>
<td>999.996E-03</td>
<td>0.000E+00</td>
<td>1.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>New_Wat_St_Str</td>
<td>q</td>
<td>0.000E+00</td>
<td>-10.000E+00</td>
<td>10.000E+00</td>
<td>1</td>
</tr>
<tr>
<td>9</td>
<td>New_Wat_St_Str</td>
<td>Ts</td>
<td>99.996E+00</td>
<td>1.000E+00</td>
<td>350.000E+00</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>New_Wat_St_Str</td>
<td>hf</td>
<td>419.595E+00</td>
<td>1.000E+00</td>
<td>2.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>New_Wat_St_Str</td>
<td>hg</td>
<td>2.676E+03</td>
<td>2.000E+03</td>
<td>5.000E+03</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>New_Wat_St_Str</td>
<td>sp_vol</td>
<td>1.671E+00</td>
<td>90.000E-06</td>
<td>300.000E+00</td>
<td>0</td>
</tr>
</tbody>
</table>
for simulation problems do not consider the calculation of stream specific volume ‘\( v \)’, except in problems which were optimised in Chapter 7 using the filterSQP code. Simulation models with ‘\( v \)’ as stream variable are presented in Sections 6.3.8, 6.5.4 - 6.5.5 and in Section 6.6. This is because the early proposal and testing of our EO models did not consider ‘\( v \)’ as stream variable. It was included for cost optimisation problems later in the research. Another important point is that, when warm-guesses were obtained for NLP optimisation, (i.e. with the addition of ‘\( v \)’ for streams), the performance of the NLAE solver still was highly efficient.

It is important to mention (as stated in Chapter 4, Section 4.1.2) that converged simulations from the NLAE solver normally require reducing both the maximum error (\( L_\infty \) norm of the scaled nonlinear equation residuals) and the maximum step size (\( L_\infty \) norm of the scaled variable step size) below user-adjustable tolerances. For these tolerances we selected \( 1.0 \times 10^{-4} \), however actual simulations produced converged \( L_\infty \) norms well below such value (e.g. down to the order of \( 1.0 \times 10^{-11} \) for a typical problem). In addition, the NLAE solver is able to use a trust region (TR) to restrict step size, which was used for some complex problems in this chapter (e.g. models in Sections 6.3.5 and 6.4.1).

For details on names and units of variables in the simulation examples below, see the relevant models in Chapter 3, Sections 3.1-3.2 and Appendices A-D.

### 6.2 Individual process streams

These are relatively simple problems involving up to 11 variables and equations (for the water/steam stream model without ‘\( v \)’ calculation). However this small simulation problems were needed in the early stages of the research, when we started testing our models.

#### 6.2.1 Water/steam stream

As stated in Chapter 3, Section 3.1.1 this model contains 11 variables and 8 equations. To solve the corresponding set of 11 independent equations and variables we need to specify 3 degrees of freedom: two for intensive variables (like \( h \) and \( P \)) and one extensive variable, mass flow.

This set of experiments reflects the behaviour of our water/steam stream model under different specifications of free variables, to define subcooled, saturated and superheated streams (see
Table 6.3). It was also useful to define proper default starting guesses for this stream which in a process flowsheet may be of any phase-type. From the water/steam stream simulation experiments we found that giving stream quality $q = 1$ and vapour fraction $\phi = 0$ as default starting guesses, along with the other stream variables having default value as shown in Table 6.1, any stream model (subcooled, saturated and superheated) converged "easily" when fixing the appropriate degrees of freedom. These simulations produced values which are in very good agreement with tabulated water/steam properties (Irvine and Liley, 1984).

Table 6.3: Water/steam streams simulations (11 equations and variables).

<table>
<thead>
<tr>
<th>iterations</th>
<th>fixed values</th>
<th>phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>T, P, F</td>
<td>superheated</td>
</tr>
<tr>
<td>10</td>
<td>T, P, F</td>
<td>subcooled</td>
</tr>
<tr>
<td>5</td>
<td>T, $q = 1.0$, F</td>
<td>saturated liquid</td>
</tr>
<tr>
<td>5</td>
<td>T, $q = 0.7$, F</td>
<td>saturated mixture</td>
</tr>
<tr>
<td>13</td>
<td>T, $q = 0.0$, F</td>
<td>saturated vapour</td>
</tr>
<tr>
<td>10</td>
<td>h, P, F</td>
<td>superheated</td>
</tr>
<tr>
<td>10</td>
<td>h, P, F</td>
<td>subcooled</td>
</tr>
<tr>
<td>10</td>
<td>h, P, F</td>
<td>saturated mixture</td>
</tr>
</tbody>
</table>

6.2.2 Multicomponent gas stream

The model for this type of stream was presented in Chapter 3, Section 3.1.3. Consider a natural gas stream containing the following hydrocarbons (Rhine and Tucker, 1991): $CH_4$, $C_2H_6$, $C_3H_8$, $nC_4H_{10}$ and $nC_5H_{12}$, identified with $C_1, \ldots, C_5$ respectively. A multicomponent gas stream with $N = 5$ (number of components) has $N + 6$ variables (11 for this example) and $N + 2 = 7$ degrees of freedom. Simulation of this stream requires the fixing of,

$$P, T, F, y_{C_1}, y_{C_2}, y_{C_3}, y_{C_4}$$

We specified $P = 2.0$ MPa, $F = 0.112$ kmol/s, $T = 300.0 \, ^\circ C$ and the independent composition for natural gas. The system with 11 variables and equations converged in only 3 iterations without using a TR for the NLAE solver. The default guesses are 'typical' values for all variables, e.g. specific entropy and enthalpy $s = 17.0 \, kJ/kmol \, K$, $h = 25 \times 10^3 \, kJ/kmol$ respectively. The converged values for these variables are $s = 7.016$ and $h = 12,683$ respectively.

---

3 we have not experimented on other combination of starting values for this stream model since the ones mentioned worked very well.

4 Meaning that the Newton step is restricted only by hard bounds on the variables.
6.3 Single units

We select a number of stand alone unit operations to show how we simulate and test individual equipment models.

In these problems the default starting guess is given as explained in Section 6.2.1 for water/steam streams. For the rest of the variables, the default guess is given by typical values, e.g. \( P = 1.5 \) MPa, \( T = 300.0 \) °C for all streams, etc.

6.3.1 Steam turbine

This example consists of a steam turbine equipment model along with its associated steam inlet and outlet streams. In the EO model we have:

<table>
<thead>
<tr>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>8 11</td>
</tr>
<tr>
<td>OUT-stream:</td>
<td>8 11</td>
</tr>
<tr>
<td>Steam turbine:</td>
<td>8 8</td>
</tr>
<tr>
<td>Total:</td>
<td>24 30</td>
</tr>
</tbody>
</table>

There are \((30 - 24) = 6\) degrees of freedom and the proposed fixed variables are:

- IN-stream: \( P_1, \ T_1, \ F_1 \)
- OUT-stream: \( P_2 \)
- Steam turbine: \( \eta_M, \ \eta_{iso} \)

By fixing these variables convergence was obtained in 11 iterations. This result was obtained without a TR.

6.3.2 Compression section of a gas turbine

For the compression section of a gas turbine, an air stream \((N_2, O_2\) mixture) has to be compressed, then we have:

<table>
<thead>
<tr>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>4 ( N + 6 = 8 )</td>
</tr>
<tr>
<td>Compressor:</td>
<td>( N + 5 = 7 ) \ 6</td>
</tr>
<tr>
<td>OUT-stream:</td>
<td>4 ( N + 6 = 8 )</td>
</tr>
<tr>
<td>Total:</td>
<td>15 22</td>
</tr>
</tbody>
</table>

Where \( N = 2 \) is the number of components. Thus there are \((22 - 15) = 7\) degrees of freedom in this case.
In this example we did the EO simulation for the compressor section of a gas turbine General Electric model LM 6000. Note that here we considered a single compression stage and the real unit is multistage (de Biasi, 1990), but the successful simulation of a whole gas turbine (Section 6.4.1) demonstrates that our considerations for the simulation of this compression section are satisfactory. A multistage compressor can easily be simulated using FMS, but since our interest was in simulating the gas turbine nominal capacity (which later is part of our CHP plants) we decided not to admit too much internal detail to this subsection simulation. The corresponding simulation was done with the following fixed variables:

| IN-stream: | F, T, P, y_{N_2} |
| Compressor: | \eta_M, \eta_{iso}, r_{cp} |

The NLAE solver converged this small problem in 6 iterations, and no TR was used.

### 6.3.3 Compressor for gas fuel

This model may represent a compressor sending natural gas e.g. to the combustion section of a gas turbine. For the compression of a gas fuel stream with \( N = 5 \) (components), described in Section 6.2.2 we have:

<table>
<thead>
<tr>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>4 ( N + 6 = 11 )</td>
</tr>
<tr>
<td>Compressor:</td>
<td>( N + 5 = 10 ) ( 6 )</td>
</tr>
<tr>
<td>OUT-stream:</td>
<td>4 ( N + 6 = 11 )</td>
</tr>
<tr>
<td>Total:</td>
<td>18 ( 28 )</td>
</tr>
</tbody>
</table>

There are \( (28 - 18) = 10 \) degrees of freedom in this case. The simulation for the stated fuel compressor was done with the following fixed variables:

| IN-stream: | F, T, P, \( y_{C_1}, y_{C_2}, y_{C_3}, y_{C_4} \) |
| Compressor: | \eta_M, \eta_{iso}, r_{cp} |

The corresponding converged solution was found without using a TR for this small system of 28 variables and equations in 7 iterations.

### 6.3.4 Gas turbine combustor premixer

We have proposed the modelling of a gas turbine combustion chamber as composed by a "pre-mixer" of fuel with air and then by a combustion reaction section (see Appendix D, Section D.2.2). Here we present the simulation of the premixing section in the combustor.
For the mixing of an air stream (having $N_1 = 2$ components) with our natural gas stream having $N_2 = 5$ components we have:

<table>
<thead>
<tr>
<th></th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-IN:</td>
<td>4</td>
<td>$N_1 + 6 = 8$</td>
</tr>
<tr>
<td>Fuel-IN:</td>
<td>4</td>
<td>$N_2 + 6 = 11$</td>
</tr>
<tr>
<td>OUT-stream:</td>
<td>4</td>
<td>$(N_1 + N_2) + 6 = 13$</td>
</tr>
<tr>
<td>Mixer:</td>
<td>$(N_1 + N_2) + 1 + 2 = 10$</td>
<td>0</td>
</tr>
<tr>
<td>Total:</td>
<td>22</td>
<td>32</td>
</tr>
</tbody>
</table>

Thus there are $(32 - 22) = 10$ degrees of freedom in this case. The simulation for the stated fuel/air mixer was done with the following fixed variables:

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-IN:</td>
<td>$F$, $T$, $P$, $y_{N_2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel-IN:</td>
<td>$F$, $T$, $y_{C_1}$, $y_{C_2}$, $y_{C_3}$, $y_{C_4}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The corresponding converged solution was found in 7 iterations. No TR was used.

### 6.3.5 Gas turbine combustion reaction section

In a gas turbine combustion chamber fuel is burned with a high excess of oxygen at high temperature and pressure (around $1,200 \degree C$ and $2.8 \text{ MPa}$ for a LM 6000).

This is a difficult sub-section to converge since the equations relating the combustion temperature and composition include dissociation reactions and are highly nonlinear (Harker and Allen, 1969), (Dixon-Lewis and Greenberg, 1975).

If the turbine inlet temperature (at the outlet of the combustor) is assumed not to exceed $1,500\degree C$, the only two equilibrium reactions that need to be considered are (Black and Hartley, 1996):

\[
\begin{align*}
CO_2 & \rightleftharpoons CO + \frac{1}{2}O_2 \\
\frac{1}{2}N_2 + \frac{1}{2}O_2 & = NO
\end{align*}
\]

This implies that the extents of reaction ($\epsilon_i$) for the remaining dissociation reactions considered in the gas turbine combustor model (see Appendix D, Section D.2.2.) are fixed at zero.

The inlet stream to this unit is a mixture of air/fuel (with $N_2$, $O_2$, $C_1, \ldots, C_5$) having $N_1 = 7$ components. We are considering the five combustion reactions of hydrocarbons as well as the

\footnote{and indeed that will happen since the projected maximum turbine inlet temperature is expected to be up to about $1,427 \degree C$ for the period 2000 - 2005 (Briesch \textit{et al.}, 1995).}
two equilibrium reactions involving \( NO \) and \( CO \), thus the OUT-stream has \( N_2 = 6 \) components \( (N_2, O_2, H_2O, CO_2, NO \) and \( CO \)). For the reactions considered we have 11 mole balance equations, 2 equilibrium relationships and the energy balance, momentum balance and fuel added equations. So in this case we have:

<table>
<thead>
<tr>
<th></th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>4</td>
<td>( N_1 + 6 = 13 )</td>
</tr>
<tr>
<td>Combustion reaction section:</td>
<td>16</td>
<td>11 + 1 + 1 + 1 = 14</td>
</tr>
<tr>
<td>OUT-stream:</td>
<td>4</td>
<td>( N_2 + 6 = 12 )</td>
</tr>
<tr>
<td>Total:</td>
<td>24</td>
<td>39</td>
</tr>
</tbody>
</table>

Thus there are \((39 - 24) = 15\) degrees of freedom. The simulation for the stated reaction section was done with the following fixed variables (many of them were the results obtained from the air/fuel premixer model from Section 6.3.4):

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>( F, T, P, y_{C_1}, y_{C_2}, y_{C_3}, y_{C_4}, y_N, y_{O_2} )</td>
</tr>
<tr>
<td>Combustion reaction section:</td>
<td>( \eta_c, \Delta P, \epsilon_8, ... \epsilon_{11} )</td>
</tr>
</tbody>
</table>

Note that the enthalpy of reaction \( AH_j(T_0) j = 1, \ldots, 11 \) used in the energy balance for this model (Appendix D, Section D.2.2.) is not considered as unit variable, but as thermopack constant.

This complex simulation problem needed the use of a \( TR = 1.0 \) for the NLAE solver for successful solution. Some of the relevant converged values include the combustion gases temperature and composition. After we selected lower bounds for mole fractions of \( 1.0 \times 10^{-11} \) and sensible starting guesses for mole fractions and temperature, the model converged in 10 iterations. From the solution of this model, the smallest mole fraction converged value is \( 4.08 \times 10^{-7} \) for \( CO \).

### 6.3.6 Expansion section of a gas turbine

The corresponding model is presented in Appendix D, Section D.2.3. This unit has two streams with \( N = 6 \) components, so we have 4 equations and \( N + 6 = 12 \) variables per stream. The expansion section model has \( N + 5 = 11 \) equations and six variables. Thus, we have \( 30 - 19 = 11 \) degrees of freedom. We gave fixed values for:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream:</td>
<td>( F, T, P, y_{N_2}, y_{O_2}, y_{CO_2}, y_{H_2O}, y_{CO} )</td>
</tr>
<tr>
<td>Expansion section:</td>
<td>( r_{ep}, \eta_M, \eta_{iso} )</td>
</tr>
</tbody>
</table>

Without using TR this problem was solved in only 6 iterations.
6.3.7 HP steam superheater

This example considers the simulation of the superheater of high pressure (HP) steam in a HRSG. We use the model for a heat recovery exchanger (given in Appendix D, Section D.3). For this unit, the source of heat is gas turbine exhaust with \( N = 6 \) components (as explained in the combustion reaction section model), so we have:

<table>
<thead>
<tr>
<th>equation</th>
<th>variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot side IN-stream:</td>
<td>( P, T, F, y_{N_2}, y_{O_2}, y_{CO_2}, y_{H_2O}, y_{CO} )</td>
</tr>
<tr>
<td>Cold side IN-stream:</td>
<td>( P, F, T )</td>
</tr>
<tr>
<td>Waste heat recovery exchanger:</td>
<td>( \eta_{HX}, \Delta P_{hs}, \Delta P_{cs}, UA, Ft )</td>
</tr>
</tbody>
</table>

In fixing the degrees of freedom for the hot side IN-stream of this heat exchange section we have considered the relevant converged values from the exhaust of the whole gas turbine simulation (Section 6.4.1).

On the other hand fixed degrees of freedom for the 'cold side' \( (P, F, T) \) as well as heat exchanger parameters: \( \Delta P_{hs}, \Delta P_{cs}, UA \) (calculated from \( UA = Q/LMTD \)), were taken from data of a real cogeneration plant (Gator-Power, 1994).

Thus, by fixing the mentioned 16 degrees of freedom and leaving the remaining default values for the other variables involved, a converged superheater model simulation was obtained in 10 iterations without the use of TR.

6.3.8 Heat recovery exchanger (for MINLP model)

For MINLP synthesis problems we used the basic heat recovery (HR) equipment model (presented in Appendix D, Section D.3), but adding the relevant logical constraints (detailed in Chapter 3, Section 3.5.4). For MINLP problems a heat recovery exchanger has associated an integer variable 'z'. \( z = 1 \) and \( z = 0 \) imply the existence (or not) of the unit. This is a problem with 82 variables and equations (taken directly from FMS list of variables). It is im-
important to mention that such value of 82 considers unit modelling variables and gas component identification numbers (used to model within FMS). This model considers water/steam streams specific volume \( \nu \).

A HP steam superheater was considered. The specifications for solving the simulation problem (and checking whether the model definition is/is not well-posed) are:

<table>
<thead>
<tr>
<th>Hot side IN-stream:</th>
<th>( P ), ( T ), ( F ), ( y_{N2} ), ( y_{O2} ), ( y_{CO2} ), ( y_{H2O} ), ( y_{CO} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cold side IN-stream:</td>
<td>( P ), ( T ), ( F )</td>
</tr>
<tr>
<td>Waste heat recovery exchanger:</td>
<td>( \eta_{HX} ), ( \Delta P_{hs} ), ( \Delta P_{cs} ), ( F_t )</td>
</tr>
<tr>
<td></td>
<td>( A ), ( U ), ( z )</td>
</tr>
</tbody>
</table>

Note that for MINLP problems this unit has an associated investment cost implying that we have \('U'\) and \('A'\) as separate variables.

For \( z = 0 \) we specify,

- \( F = 1.0 \times 10^{-7} \) kmol/s for hot side IN-stream (equal to its lower bound). This is to avoid numerical difficulties with mole balance equations for \( F = 0 \).
- \( F = 0.0 \) kg/s for cold side stream (equal to its lower bound)
- \( A = 0 \) m\(^2\)

With these specifications the model converged quite well in 9 iterations without using a TR, e.g. in the solution we got \( Q = 0.0 \), cost of HR = 0.0, \( T_1 = T_2 \) for both streams, etc.

For \( z = 1 \) we specify,

- \( F = 4.39 \) kmol/s for hot side stream
- \( F = 10.31 \) kg/s for cold side stream
- \( A = 877.7 \) m\(^2\)

With these specifications the model converged in 9 iterations without using a TR.

Note that in MINLP problems (Chapter 8) we free \('A'\) and all stream variables, for both cold and hot streams passing through a heat recovery exchanger with free integer variable \('z'\).
For this simulation problem the upper bound of slack variables associated with logical constraints (see Chapter 3, Section 3.5.4) was selected to be equal to the upper bound for the continuous relevant variable within the logical c/s.

With this set of numerical experiments we assessed that the HR model will have a solution with fixed $z = 0$ and $z = 1$, so we expect that the integer relaxations in the MINLP solution method (when integer variables $z$ are considered continuous i.e. $0 \leq z \leq 1$) will also have a solution for this model.

6.3.9 Multicomponent gas streams mixer/splitter

This EO simulation examples using the NLAE solver without trust region were done to assess the model described in Appendix D, Section D.10.

**Combustor premixer for a SIGT**

The combustor of steam injected gas turbines (SIGT) is modelled considering a premixer of steam/fuel/air. The mixer has a steam-IN, an air-IN and a natural gas-IN streams with $N_1 = 1$, $N_2 = 2$, $N_3 = 5$ components respectively. The corresponding modelling variables and equations are:

<table>
<thead>
<tr>
<th></th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam-IN:</td>
<td>4</td>
<td>$N_1 + 6 = 1 + 6 = 7$</td>
</tr>
<tr>
<td>Air-IN:</td>
<td>4</td>
<td>$N_2 + 6 = 2 + 6 = 8$</td>
</tr>
<tr>
<td>Fuel-IN:</td>
<td>4</td>
<td>$N_3 + 6 = 5 + 6 = 11$</td>
</tr>
<tr>
<td>OUT-Stream:</td>
<td>4</td>
<td>$(N_1 + N_2 + N_3) + 6 = 14$</td>
</tr>
<tr>
<td>Mixer:</td>
<td>$(N_1 + N_2 + N_3) + 1 + 3 = 12$</td>
<td>0</td>
</tr>
<tr>
<td>Total:</td>
<td>28</td>
<td>40</td>
</tr>
</tbody>
</table>

Thus there are $(40 - 28) = 12$ degrees of freedom. The simulation for the stated steam/fuel/air mixer was done with the following fixed variables:

| Steam-IN: | F, T, $y_{N2}$ |
| Air-IN:   | F, T, P, $y_{N2}$ |
| Fuel-IN:  | F, T, $y_{C_1}$, $y_{C_2}$ |
|           | $y_{C_3}$, $y_{C_4}$ |

The corresponding converged solution was found in 6 iterations.
Steam/fuel/air splitter

Taking the independent variables of the OUT-stream from the above example for the IN-stream of a splitter with 3-OUT streams constituted this example. Now \( N = 8 \) is the total number of components entering the splitter and \( N_{OUT} = 3 \) is the number of OUT-streams. So we have:

<table>
<thead>
<tr>
<th></th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN-stream: ( N + 6 )</td>
<td>4</td>
<td>( N + 6 = 8 + 6 = 14 )</td>
</tr>
<tr>
<td>3 OUT-streams: ( 4(3) )</td>
<td>12</td>
<td>( 3 \ (N + 6) = 42 )</td>
</tr>
<tr>
<td>Mixer: ( N + 1 + 3 + 2+ ) ( (N_{OUT} - 1) \ (N - 1) )</td>
<td>28</td>
<td>0</td>
</tr>
<tr>
<td>Total :</td>
<td>44</td>
<td>56</td>
</tr>
</tbody>
</table>

We have \( (56 - 44) = 12 \) degrees of freedom. The simulation for the stated steam/fuel/air splitter was done with the following fixed variables:

| IN-stream: \( F, \ T, \ P, \ y_C, \ y_C2, \ y_C3, \ y_C4, \ y_C5, \ y_N, \ y_O, \) |
| OUT-stream 1: \( F \) |
| OUT-stream 2: \( F \) |

This example was solved in 6 iterations.

Gas turbine exhaust splitter with 8 OUT-streams

In the MINLP model in Chapter 3, Section 3.5.4, the gas turbine exhaust (in the superstructure) should be split into as many as potential waste heat exchangers that may exist. In this case we have 8 HR exchangers.

In general the gas turbine (IN-stream) for this splitter should be fully specified by giving \( N + 2 \) independent variables and the molar flow of all except one of the OUT-streams.

The construction of this model in FMS required 176 variables and equations. After model verification with the EA this problem was solved in 5 iterations.
6.4 Complex unit operations

6.4.1 A commercial gas turbine

The model for this equipment is shown in Appendix D, Section D.2. We first simulated this equipment in its individual equipment sections (see Sections 6.3.2 - 6.3.6), due mainly to the complexity of the combustion chamber model.

Once partial solutions were obtained for each sub-section, we easily constructed and solved the model for simulation of the full gas turbine (using FMS) by interconnecting the gas turbine sub-sections.

A General Electric LM 6000 gas turbine was simulated. This included some non-idealities described by the parameters shown in Table 6.4 (Rodriguez-Toral, 1993). The numbers of variables and equations for a gas turbine model are as shown in Table 6.5. In this case there are \((109 - 83) = 26\) degrees of freedom for the whole gas turbine in open cycle. We fixed the extent of reactions to zero for dissociations not likely to occur at gas turbine highest combustion

<table>
<thead>
<tr>
<th>Pressure drop in combustion chamber:</th>
<th>(\Delta P_{cc} \leq 3.0%) of inlet (P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Efficiency on mechanical transmission:</td>
<td>(\eta_{mt} \geq 99.0%)</td>
</tr>
<tr>
<td>Combustor thermal losses:</td>
<td>(T_{loss} = 2.0%)</td>
</tr>
</tbody>
</table>

Table 6.4: Non-ideality parameters for the simulation of gas turbines.

<table>
<thead>
<tr>
<th></th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel-IN compressor:</td>
<td>4</td>
<td>11</td>
</tr>
<tr>
<td>Fuel compressor:</td>
<td>10</td>
<td>6</td>
</tr>
<tr>
<td>Fuel-OUT compressor:</td>
<td>4</td>
<td>11</td>
</tr>
<tr>
<td>Air-IN compressor section:</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Compressor section:</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>Air-OUT compressor section:</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Air/fuel mixer:</td>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>Air/fuel mixer OUT-stream:</td>
<td>4</td>
<td>13</td>
</tr>
<tr>
<td>Combustion chamber:</td>
<td>16</td>
<td>14</td>
</tr>
<tr>
<td>Expansion section IN-stream:</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>Expansion section:</td>
<td>11</td>
<td>6</td>
</tr>
<tr>
<td>Exhaust gas:</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>Power output equation:</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Total for the system:</td>
<td>83</td>
<td>109</td>
</tr>
</tbody>
</table>

Table 6.5: Modelling variables and equations for a gas turbine.
temperature as explained in Section 6.3.5. For the simulation of a General Electric LM 6000 gas turbine we also fixed the variables shown in Table 6.6 where subscripts 'f' and 'a' refer to fuel and air respectively; 'y' is the mole fraction for a given component and η are the efficiencies for isentropic conditions (η_iso), mechanical efficiency (η_M), combustion efficiency (η_c), and mechanical transmission efficiency for the turbine-compressor shaft (η_mt). 'τ_c' and 'τ_e' are the compressor and expander pressure ratios.

The full gas turbine simulation converged in 32 iterations using a TR = 1.0 for the NLAE solver. For this simulation we used the default initial values for all the variables including molar flows, \( H, h_{gas}, s_{gas} \) for all the gas streams, but carefully chose starting guesses for the combustion chamber \( T \), and for the combustion products composition.

The simulation was successful because by fixing a few independent variables the model gave the key parameters for the modelled gas turbine: the power output, the quantity of fuel consumed, the combustor temperature and composition and for further exhaust heat recovery the exhaust mass flow, temperature and composition. The exhaust gas composition obtained is in good agreement with other investigations where a sequential modular simulation of gas turbines using HYSIM was performed (Rodríguez-Toral, 1993).

Table 6.6: Fixed variables for the simulation of a gas turbine.

<table>
<thead>
<tr>
<th>Fuel-IN to compressor:</th>
<th>( P_f, ) ( T_f, ) ( F_f, ) ( y_{C1}, ) ( y_{C2}, ) ( y_{C3}, ) ( y_{C4} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel compressor:</td>
<td>( \eta_{iso}, ) ( \eta_M )</td>
</tr>
<tr>
<td>Air-IN compressor section:</td>
<td>( P_a, ) ( T_a, ) ( F_a, ) ( y_{N2} )</td>
</tr>
<tr>
<td>Gas turbine compressor section:</td>
<td>( \eta_{iso}, ) ( \eta_M, ) ( \tau_e )</td>
</tr>
<tr>
<td>Combustion chamber:</td>
<td>( \epsilon_8, ) ( \epsilon_9, ) ( \epsilon_{10}, ) ( \epsilon_{11}, ) ( \eta_c, ) ( \Delta P_{cc} )</td>
</tr>
<tr>
<td>Expansion section:</td>
<td>( \eta_{iso}, ) ( \eta_M, ) ( \tau_e )</td>
</tr>
<tr>
<td>Power output equation:</td>
<td>( \eta_{mt} )</td>
</tr>
</tbody>
</table>

Table 6.7: Comparison of simulation results for a gas turbine LM 6000 in simple cycle.

<table>
<thead>
<tr>
<th></th>
<th>Manufacturer’s specifications</th>
<th>EO simulation</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shaft output:</td>
<td>40,265.0 kW</td>
<td>40,265.0 kW</td>
<td>0.0</td>
</tr>
<tr>
<td>Thermal efficiency:</td>
<td>41.0%</td>
<td>40.98%</td>
<td>0.032</td>
</tr>
<tr>
<td>High pressure turbine inlet:</td>
<td>1,265.5 °C</td>
<td>1,265.0 °C</td>
<td>0.039</td>
</tr>
<tr>
<td>Exhaust gas flow:</td>
<td>117.5 kg/s</td>
<td>116.815 kg/s</td>
<td>0.55</td>
</tr>
<tr>
<td>Exhaust gas temperature:</td>
<td>473.0 °C</td>
<td>473.084 °C</td>
<td>0.017</td>
</tr>
</tbody>
</table>
A comparison is shown in Table 6.7 between the manufacturer's values for LM 6000 gas turbine (de Biasi, 1990) and the ones obtained in this simulation. It is important to mention that the EO simulation produced very good agreement with the commercial unit due to the fact that we adjusted efficiencies (in expander, compressor and combustion chamber) accordingly.

6.4.2 HRSG (subsections simulation)

In this and the next sub-section we present the simulation of a heat recovery steam generator (HRSG) having three steam pressure levels as shown in Fig. 6.2. This equipment is currently in operation (Gator-Power, 1994).

The high pressure (HP) heat recovery sections involve three economisers, one evaporator and three superheaters. On the other hand the intermediate pressure (IP) steam system within this HRSG has one exchange section for the economiser, one for the evaporator and one for the superheater. These heat recovery units are not "consecutive", in that they are not immediately adjacent to one another for the IP subsystem (see Fig. 6.2). Finally, the low pressure (LP) steam system involves steam generation for deaeration and for heat load purposes. For each pressure steam level the "blow down" (purge) from the steam drums is also modelled.

The EO simulation of the HRSG shown in Figure 6.2 proved to be a difficult problem. We needed to solve separate subsystems first. In our experience it was best to include at most one steam drum in each sub-system simulation, for ease of solution. Thus we decomposed the HRSG into four subsystems as depicted in Fig. 6.3. Each contains also at most one evaporator section and are simulated below.

**HP steam superheaters and HP evaporator simulation**

This subsection is shown in Fig. 6.4 and consists of three HP steam superheating sections, a desuperheater (using water), the possibility of using a duct burner (currently not simulated) and the HP steam generator with its associated steam drum.

The numbers of variables and equations for this sub-section are shown in Table 6.8. Thus there are \((214 - 181) = 33\) degrees of freedom that were fixed by specifying the variables in Table 6.9. Our general policy for specifying variables in a HRSG sub-section was to fix:
CHAPTER 6. SIMULATION RESULTS AND DISCUSSION

Figure 6.2: HRSG with three steam pressure levels.
Figure 6.3: Subsections for the HRSG simulation.
Figure 6.4: HP superheaters as well as its HP evaporator.

Table 6.8: Modelling variables and equations for the HRSG subsection including HP steam superheaters and HP evaporator.

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>11</td>
<td>11 (8) = 88</td>
</tr>
<tr>
<td>Gas streams:</td>
<td>5</td>
<td>5 (4) = 20</td>
</tr>
<tr>
<td>Heat recovery sections:</td>
<td>4</td>
<td>4 (14) = 56</td>
</tr>
<tr>
<td>Splitters:</td>
<td>1</td>
<td>1 (5) = 5</td>
</tr>
<tr>
<td>Mixers:</td>
<td>1</td>
<td>1 (4) = 4</td>
</tr>
<tr>
<td>Steam drums:</td>
<td>1</td>
<td>1 (8) = 8</td>
</tr>
<tr>
<td>Total:</td>
<td>23</td>
<td>181</td>
</tr>
</tbody>
</table>

- independent variables for the hot stream entering (here, exhaust from a gas turbine);
- independent variables for the liquid-IN streams (in this case, sub-cooled liquid to the steam Drum and water to the desuperheater, see Fig. 6.4);
- design variables for each item of heat recovery equipment ($\eta_{HX}$, the efficiency in heat recovery; $\Delta P_h$ and $\Delta P_c$, the pressure drop for the hot side and for the cold side; $UA$, the product of overall heat transfer coefficient and the heat transfer area; and $F_{L}$, the $LMTD$ correction factor. For a given simulation these variables are given for each item of heat recovery equipment, e.g. for a HP superheater); and
- for evaporation sections the quality ‘$q$’ of the steam produced.

In our experience the use of appropriate bounds on steam temperatures was beneficial. The upper bound on steam stream temperatures was given as 450 °C \(^6\) while the exhaust gas could

\(^6\) In fact we could have selected any upper bound above 383.7 °C, which is the HP superheated steam $T$ for the real plant, but smaller than say 468 °C to allow feasible driving forces in heat exchange.
be around 473 °C. With these fixed variables and bounds on steam temperatures the simulation converged in 12 iterations without the use of TR.

We used $Q = 8.0 \times 10^3$ kW as the starting guess for all the heat exchanger duties. This value is about half of the highest heat load of any heat exchanger in this HRSG section and was used instead of the default value, $Q = 50.0 \times 10^3$ kW. The remaining variables kept their default initial guesses.

The simulation produced satisfactory numerical results as shown in Table 6.10 where we compare some parameters given for the existing design (Gator-Power, 1994) at The University of Florida’s cogeneration plant with those obtained in our simulation. Our results are close to those of the real plant, for those variables which were reported for the real plant. Our model contains many more modelling variables which are not reported for the real plant, e.g. water/steam enthalpies, entropies, steam quality, etc. for every water/steam stream.

**Intermediate pressure (IP) superheater, HP economisers 1 and 2 and IP evaporator simulation**

The next sub-section of the HRSG consists of the HP economisers 1 and 2, the IP steam generator and IP superheater. A schematic diagram is shown in Fig. 6.5.

For this sub-section the number of variables and equations are shown in Table 6.11. There were $(203 - 169) = 34$ degrees of freedom, fixed by specifying the variables in Table 6.12, chosen according to the principles outlined above. Water/steam temperature upper bounds were set to 300.0 °C and default values were used for heat loads (1,000.0 kW) and for temperatures (100.0 °C). The simulation of this sub-section converged in 21 iterations, and produced satisfactory...
Table 6.10: Comparison of results for the simulation of the HRSG subsection including HP steam superheaters and HP evaporator.

<table>
<thead>
<tr>
<th></th>
<th>Existing design U. of Florida</th>
<th>EO simulation</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP superheater No.1</td>
<td>1,526.8 kW</td>
<td>1,581.0 kW</td>
<td>3.5</td>
</tr>
<tr>
<td>Heat load</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>422.2/411.6</td>
<td>422.2/410.9</td>
<td>0.0/0.17</td>
</tr>
<tr>
<td>Steam T in/out °C</td>
<td>326.1/382.2</td>
<td>322.6/381.6</td>
<td>1.1/0.16</td>
</tr>
<tr>
<td>HP superheater No.2</td>
<td>451.3 kW</td>
<td>477.6 kW</td>
<td>5.8</td>
</tr>
<tr>
<td>Heat load</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>411.6/408.3</td>
<td>410.9/407.4</td>
<td>0.17/0.22</td>
</tr>
<tr>
<td>Steam T in/out °C</td>
<td>330.5/346.6</td>
<td>326.0/343.1</td>
<td>1.3/1.0</td>
</tr>
<tr>
<td>HP superheater No.3</td>
<td>2,230.2 kW</td>
<td>2,287.0 kW</td>
<td>2.5</td>
</tr>
<tr>
<td>Heat load</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>408.3/392.7</td>
<td>407.4/390.9</td>
<td>0.22/0.45</td>
</tr>
<tr>
<td>Steam T in/out °C</td>
<td>264.4/330.5</td>
<td>263.8/326.0</td>
<td>0.45/1.3</td>
</tr>
<tr>
<td>HP boiler</td>
<td>16,912.9 kW</td>
<td>16,861.0 kW</td>
<td>0.3</td>
</tr>
<tr>
<td>Heat load</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>392.7/272.7</td>
<td>390.9/267.3</td>
<td>0.45/1.9</td>
</tr>
<tr>
<td>Water/steam T in/out °C</td>
<td>264.4/264.4</td>
<td>263.7/263.7</td>
<td>0.26/0.26</td>
</tr>
</tbody>
</table>

Table 6.11: Modelling variables and equations for the HRSG subsection including HP economisers 1 and 2, IP superheater, IP evaporator and its steam drum.

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>10 (8) = 80</td>
<td>10 (11) = 110</td>
</tr>
<tr>
<td>Gas streams:</td>
<td>5 (4) = 20</td>
<td>5 (12) = 60</td>
</tr>
<tr>
<td>Heat recovery sections:</td>
<td>4 (14) = 56</td>
<td>4 (8) = 32</td>
</tr>
<tr>
<td>Splitters:</td>
<td>1 (5) = 5</td>
<td>0</td>
</tr>
<tr>
<td>Steam drum:</td>
<td>1 (8) = 8</td>
<td>1 (1) = 1</td>
</tr>
<tr>
<td>Total:</td>
<td>21</td>
<td>169</td>
</tr>
</tbody>
</table>

Table 6.12: Fixed variables for the HRSG subsection including HP economisers 1 and 2, IP superheater, IP evaporator and its steam drum.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \eta_{HX} ), ( \Delta P_{hs} ), ( \Delta P_{cs} ), ( UA ), ( F_t )</td>
<td>( P ), ( T ), ( F ), ( y_{N2} ), ( y_{O2} )</td>
<td>( y_{CO2} ), ( y_{H2O} ), ( y_{CO} )</td>
<td>( \eta_{HX} ), ( \Delta P_{hs} ), ( \Delta P_{cs} ), ( UA ), ( F_t )</td>
<td>( P ), ( T ), ( F )</td>
<td>( q = 0.0 )</td>
<td>( F )</td>
<td>( F )</td>
</tr>
</tbody>
</table>
results as shown in Table 6.13.

![Diagram of HP economisers 1 and 2, IP superheater, IP evaporator and its steam drum.]

Figure 6.5: HP economisers 1 and 2, IP superheater, IP evaporator and its steam drum.

Table 6.13: Simulation results for the IP superheater, HP economisers 1 and 2 as well as IP evaporator.

<table>
<thead>
<tr>
<th></th>
<th>Existing design U. of Florida</th>
<th>EO simulation</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>IP superheater</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat load</td>
<td>284.3 kW</td>
<td>288.5 kW</td>
<td>1.46</td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>272.7/271.1</td>
<td>272.7/270.6</td>
<td>0.0/0.18</td>
</tr>
<tr>
<td>Steam T in/out °C</td>
<td>170.5/210.0</td>
<td>172.5/207.5</td>
<td>1.2/1.2</td>
</tr>
<tr>
<td>HP economiser No.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat load</td>
<td>1,471.2 kW</td>
<td>1,476.0 kW</td>
<td>0.32</td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>271.1/260.5</td>
<td>270.6/259.6</td>
<td>0.18/0.36</td>
</tr>
<tr>
<td>Water T in/out °C</td>
<td>227.7/257.7</td>
<td>227.2/257.3</td>
<td>0.22/0.16</td>
</tr>
<tr>
<td>HP economiser No.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat load</td>
<td>3,669.2 kW</td>
<td>3,654.0 kW</td>
<td>0.41</td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>260.5/233.8</td>
<td>259.6/232.3</td>
<td>0.36/0.64</td>
</tr>
<tr>
<td>Water T in/out °C</td>
<td>147.7/227.7</td>
<td>-147.7/227.2</td>
<td>0.0/0.22</td>
</tr>
<tr>
<td>IP boiler</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat load</td>
<td>6,752.3 kW</td>
<td>6,736.0 kW</td>
<td>0.24</td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>233.8/184.4</td>
<td>232.3/181.6</td>
<td>0.64/1.5</td>
</tr>
<tr>
<td>Water/steam T in/out °C</td>
<td>170.5/170.5</td>
<td>171.5/172.5</td>
<td>0.58/1.2</td>
</tr>
</tbody>
</table>
LP steam drum and LP evaporator simulation

The third sub-section of the HRSG consists of the LP steam generator as illustrated in Fig. 6.6. Enumerating the variables and equations in a way similar to previous HRSG-subsections, we found that there are \((99 - 83) = 16\) degrees of freedom for this sub-section. 16 independent variables were specified using the same approach as in the previous examples.

This EO simulation converged in only 8 iterations, from a starting guess in which all \(T = 100.0 \, ^\circ C\) and \(Q = 1,000.0 \, kW\). Again, comparing a number of key parameters of the real plant with values from the simulation (see Table 6.14) we observed very good agreement (within 1%).

![Figure 6.6: LP steam drum and LP evaporator.](image)

Table 6.14: Simulation results for the LP evaporator.

<table>
<thead>
<tr>
<th></th>
<th>Existing design U. of Florida</th>
<th>EO simulation</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>LP boiler:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat load</td>
<td>3,897.8 kW</td>
<td>3,864.0 kW</td>
<td>0.87</td>
</tr>
<tr>
<td>Exhaust T in/out °C</td>
<td>184.4/156.1</td>
<td>184.4/155.1</td>
<td>0.0/0.64</td>
</tr>
<tr>
<td>Water/steam T in/out °C</td>
<td>138.3/138.3</td>
<td>138.0/139.3</td>
<td>0.21/0.72</td>
</tr>
</tbody>
</table>
IP economiser and HP economiser No. 3 simulation

The last sub-section for the simulation of the HRSG has two economiser heat recovery sections, one for IP and another for HP as can be seen in Fig. 6.7. For this sub-section we found \( (96 - 72) = 24 \) degrees of freedom which were fixed for the simulation problem using the same approach as above.

This EO simulation converged in 9 iterations without the use of a TR.

Again, the starting guess set all \( T = 100.0^\circ\text{C} \) and \( Q = 1,000.0 \text{ kW} \), with all remaining variables having their default starting guess. The simulation produced satisfactory results when compared with the real plant, as shown in Table 6.15.

### 6.4.3 HRSG (complete unit)

Once we had simulated the HRSG sub-sections and obtained accurate results, we proceeded with the simulation of the whole HRSG. The enumeration of modelling variables and equations is presented in Table 6.16. This model had 11 heat recovery equipment items.

![Figure 6.7: IP economiser and HP economiser No. 3.](image-url)
The complete HRSG model has \((543 - 469) = 74\) degrees of freedom. These degrees of freedom were fixed with the same choice of specified variables as in the separate HRSG sub-sections already simulated.

As in the smaller models and before using the sparse NLAE solver, we ran the model of the HRSG through the EA. With the 74 specifications the EA found no superfluous equations nor free variables in the model.

Values for the specified variables were available either from the original designer (Gator-Power, 1994) or from the sub-section simulations above. Some of the previous results were used as starting guesses.

The full HRSG model converged in 42 iterations, without the use of a trust region.

We observed that variables like heat loads, hot gas and water/steam temperatures through each of the 11 heat recovery units again are in good agreement with the design values found in the simulation of HRSG sub-sections.

| Table 6.15: Simulation results for the IP economiser and the HP economiser No. 3. |
|-----------------------------|-----------------------------|-----------------------------|
|                             | Existing design U. of Florida | EO simulation | % error |
| IP economiser               |                             |               |        |
| Heat load                   | 583.2 kW                    | 569.8 kW      | 2.3    |
| Exhaust T in/out °C         | 156.1/151.6                 | 155.1/150.7   | 0.64/0.59 |
| Water T in/out °C           | 110.0/152.2                 | 110.0/151.5   | 0.0/0.46 |
| HP economiser No. 3         |                             |               |        |
| Heat load                   | 3,551.9 kW                  | 3,554.0 kW    | 0.06   |
| Exhaust T in/out °C         | 151.1/125.0                 | 150.7/123.6   | 0.26/1.12 |
| Water T in/out °C           | 65.5/147.2                  | 65.5/147.3    | 0.0/0.07 |

| Table 6.16: Modelling variables and equations for the HRSG. |
|-----------------------------|-----------------------------|-----------------------------|
|                             | Units | equations | variables |
| Water/steam streams:        | 28    | 28 \((8) = 224\) | 28 \((11) = 308\) |
| Gas streams:                | 12    | 12 \((4) = 48\) | 12 \((12) = 144\) |
| Heat recovery sections:     | 11    | 11 \((14) = 154\) | 11 \((8) = 88\) |
| Splitters:                  | 3     | 3 \((5) = 15\) | 0 |
| Mixers:                     | 1     | 1 \((4) = 4\) | 0 |
| Steam drums:                | 3     | 3 \((8) = 24\) | 3 \((1) = 3\) |
| Total:                      | 58    | 469        | 543       |
The results of the whole HRSG with its 11 heat recovery sections were used to prepare a data file in suitable format for FMS, so as to provide a starting guess for the whole HRSG when running later simulations of the cogeneration plant containing the HRSG.

6.5 Plant sections

6.5.1 Air compression system

This is a plant-section of 'the MASSBAL problem', a CHP plant optimised in Chapter 7, Section 7.1. The corresponding flowsheet is shown there and in Fig. 6.8 for easy reference. For the air compression system we have:

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air streams: 6</td>
<td>6 (3) = 18</td>
<td>6 (6) = 36</td>
</tr>
<tr>
<td>Compressors: 2</td>
<td>2 (6) = 12</td>
<td>2 (6) = 12</td>
</tr>
<tr>
<td>Splitters: 1</td>
<td>1 (5) = 5</td>
<td>0</td>
</tr>
<tr>
<td>Mixers: 1</td>
<td>1 (4) = 4</td>
<td>0</td>
</tr>
<tr>
<td>Total: 10</td>
<td>39</td>
<td>48</td>
</tr>
</tbody>
</table>

Thus there were (48 − 39) = 9 degrees of freedom. We used the following fixed variables:

IN-stream to air-splitter: $P$, $T$, $F$

IN-stream to RECIP.COMP: $F$

OUT-stream of TC.COMP: $P$

TC.COMP: $\eta_M$, $\eta_{iso}$

RECIP.COMP: $\eta_M$, $\eta_{iso}$

Figure 6.8: The air system in the MASSBAL problem.
6.5.2 Gas turbine and HRSG

Once the gas turbine and the HRSG had been individually simulated it was easy to construct the combined model for these two plant sections. The exhaust gas from the gas turbine is connected as the source of heat for steam generation. Fig. 6.9 shows the combined flowsheet.

The previous gas turbine simulation (shown in Section 6.4.1) did not include steam injection unlike the one in the real cogeneration plant. However, the gas turbine is now modelled as using steam injection.

As a result of adding steam injection as well as the stream connection from the gas turbine exhaust to the HRSG (see Fig. 6.9) the number of modelling variables and equations is changed as in Table 6.17.

There are \((648 - 554) = 94\) degrees of freedom which were fixed for the simulation. The simulation used a warm starting guess formed from the results of the simulations of sub-sections, and converged in 25 iterations without using a TR.

As in the sub-sections simulations the results showed very good agreement with the real plant for the variables reported for the original design (Gator-Power, 1994), for example the maximum % error from the simulation for the next generic variables is:

- heat loads: 4.28%
- water/steam streams temperatures: 0.92%
- gas turbine exhaust temperatures throughout the HRSG: 0.48%
- gas turbine power produced: 0.012%

Table 6.17: Modelling variables and equations for the gas turbine (with steam injection) and the HRSG.

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas turbine:</td>
<td>1</td>
<td>83 + 6 = 89</td>
</tr>
<tr>
<td>HRSG:</td>
<td>1</td>
<td>469 - 4 = 465</td>
</tr>
<tr>
<td>Total :</td>
<td>2</td>
<td>554</td>
</tr>
</tbody>
</table>
Figure 6.9: Gas turbine and HRSG.
Figure 6.10: Water/steam distribution system.
6.5.3 Water/steam distribution system

The cogeneration plant selected for testing our EO approach (Gator-Power, 1994) has a water/steam distribution system as shown in Fig. 6.10. The water/steam distribution system consists of HP and IP steam demands as well as all the associated auxiliary equipment like pumps, deaerator, water/water heat exchangers, tanks and valves.

We solved this simulation problem in two sub-systems (whose results are not detailed here) and then the results for variables of the converged partial solutions were used to get a starting guess good enough for the simulation of the complete distribution system.

For the water/steam distribution system the number of modelling variables and equations is shown in Table 6.18.

Table 6.18: Modelling variables and equations for the water/steam distribution system.

<table>
<thead>
<tr>
<th>Unit</th>
<th>Variables</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>48</td>
<td>48 (8) = 384</td>
</tr>
<tr>
<td>Condenser load:</td>
<td>2</td>
<td>2 (3) = 6</td>
</tr>
<tr>
<td>Mixers:</td>
<td>5</td>
<td>5 (4) = 20</td>
</tr>
<tr>
<td>Splitters:</td>
<td>9</td>
<td>9 (5) = 45</td>
</tr>
<tr>
<td>Pumps:</td>
<td>4</td>
<td>4 (8) = 32</td>
</tr>
<tr>
<td>Water/water heat exchanger:</td>
<td>2</td>
<td>2 (9) = 18</td>
</tr>
<tr>
<td>Valves:</td>
<td>9</td>
<td>9 (3) = 27</td>
</tr>
<tr>
<td>Deaerator:</td>
<td>1</td>
<td>1 (11) = 11</td>
</tr>
<tr>
<td>Total:</td>
<td>80</td>
<td>543</td>
</tr>
</tbody>
</table>

There are \((594 - 543) = 51\) degrees of freedom for the HP/IP/LP water/steam distribution system. Values for 51 specified variables were selected using designer's information (where available) and the partial simulation solutions. The model was checked for satisfactory specification structure using the EA and the simulation problem was then solved in 15 iterations by the sparse solver without using a TR.

6.5.4 Rankine cycle-part of a combined cycle

The steam system part of a combined cycle with two steam pressure levels is illustrated in Fig. 6.11. This simulation was done in order to provide a warm-guess for the economic optimisation problem in Chapter 7, Section 7.5.1. Note that in the related economic optimisation problem (Chapter 7, Section 7.5.1) this model considers 'U', 'A' as separate variables and adds
Figure 6.11: Steam system of a combined cycle with two steam pressure levels.
‘v’ for water/steam and air single-component streams. In addition, we model the condensate tank (in Fig. 6.11) simply as a mixer unit. This subsystem has variables and equations as shown in the table below:

<table>
<thead>
<tr>
<th>Units equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams 29 (9) = 261 29 (12) = 348</td>
<td></td>
</tr>
<tr>
<td>Steam turbines 2 2 (8) = 16 2 (8) = 16</td>
<td></td>
</tr>
<tr>
<td>Air-cooled condenser 1 1 (14) = 14 1 (13) = 13</td>
<td></td>
</tr>
<tr>
<td>Air streams 2 2 (4) = 8 2 (7) = 14</td>
<td></td>
</tr>
<tr>
<td>Pumps 4 4 (8) = 32 4 (8) = 32</td>
<td></td>
</tr>
<tr>
<td>Splitters 4 4 (5) = 20 0</td>
<td></td>
</tr>
<tr>
<td>Mixers 3 3 (4) = 12 0</td>
<td></td>
</tr>
<tr>
<td>Water/water heat exchanger 1 (10) = 10 1 (9) = 9</td>
<td></td>
</tr>
<tr>
<td>Valves 4 4 (3) = 12 4 (1) = 4</td>
<td></td>
</tr>
<tr>
<td>Deaerator 1 1 (11) = 11 1 (11) = 11</td>
<td></td>
</tr>
</tbody>
</table>

There are (447 – 396) = 51 degrees of freedom for the model of this subsystem. We fixed the appropriate variables so as to get a fully constrained model (verified with the EA) and give no further details since the fixed variables are selected with the same logic as in the previous simulation models.

In an early experience with this simulation model, among the fixed variables we set \( F = 0.0 \) for the split stream going to valve \( V4 \) (see Fig. 6.11). After model verification with the EA, the sparse NLAE solver converged to a solution (in 7 iterations) where all the flowsheet variables got correct values, except valve \( V4 \) OUT-stream which got a spurious temperature. This is because the specification of \( F = 0 \) for valve \( V4 \) IN-stream produced one singular equation: the valve \( V4 \) OUT-stream enthalpy flow (given by \( F_2h_2 \)), actually identified by the NLAE solver.

After this experience with \( F = 0 \) we fixed water mass flow through valve \( V4 \) (Fig. 6.11) with \( F_1 = 1.0 \times 10^{-8} \) kg/s and the model for the Rankine cycle-part of a combined cycle converged in 9 iterations without using a TR.

### 6.5.5 Hyperstructure for the synthesis of HP steam superheaters

We consider now the hyperstructure used for the MINLP synthesis problem presented in Chapter 8, Section 8.2. This model contains 3 HP superheaters and a HP evaporator as well as the relevant mixers/splitters in the cold and hot side superstructures. See Fig. 6.12 where we show the ‘cold side’ superstructure only. Details on how we model the ‘hot side’ superstructure are given in Chapter 3, Section 3.5.3.
For this simulation model we consider the HR exchangers operating in series, i.e. hot gas goes to HP superheater 'HP shtr 1' then to 'HP shtr 2' and later to 'HP shtr 3' where it passes to the HP evaporator (see Fig. 6.12). We include water/steam stream specific volume 'v'.

In this problem we did not ‘manually’ construct a table showing the number of variables and equations (as in some of the previous examples), but once the model was defined and assessed (with the EA) we took from FMS the size of this problem (containing 514 variables and equations). The fixed variables are:

| Hot side IN-stream: (from gas turbine exhaust) | $P$, $T$, $F$, $y_{N_2}$, $y_{O_2}$, $y_{CO_2}$, $y_{H_2O}$, $y_{CO}$ |
|---|---|---|---|---|
| HP water to steam drum: | $P$, $F = 10$ |
| Steam drum: | $\Delta T_{Drum}$ |
| HP steam through HR exchangers: | $F = 10$ |
| Other independent steam $F$ from/to splitters/mixers | $F = 0$ |
| HP superheaters OUT-stream (superheated steam): | $T$ |
| Steam drum blow-down water: | $F$ |
| Waste heat recovery exchangers: | $\eta_{HX}$, $\Delta P_{hs}$, $\Delta P_{cs}$, $F_t$, $UA$, $U$, $z$ |

Note that our superstructure involves a multiple-recycle flowsheet. For the analysis of this model we use the EA with:

- Equation reordering by increasing initial row count (Morton and Collingwood, 1998).
- No block finding method.

Then for this problem the EA identified no free variables, but the following redundant equations: One of the momentum balances for mixer ‘MCS 6’ (Fig. 6.12); two of the momentum balances for mixer ‘MCS 7’; and two of the momentum balances for mixer ‘MCS 8’. See Fig. 6.12 where the streams producing redundant momentum balances are marked with dotted lines.

Other redundant equations were: all $\Delta P$ for cold and hot streams through HR equipments (fixed as 0.0 to satisfy recycles momentum balances around mixers/splitters).

For solving this problem with the above-mentioned superfluous equations we use the following options for the NLAE solver (Morton, 1997): a default step = 0.0; a variable chopping method for step restriction; a reordering option by a Markowitz-like method; no block solution option; and no TR.

---

7 These and other parameters for the EA are chosen in a control file (Morton and Collingwood, 1998).
Having a warm-guess for two of the superheaters and for mixer 'MCS 8' (which supplies superheated steam), but default values for other variables the NLAЕ solver converged this problem in 7 iterations without the use of TR.

6.6 Whole utility systems

Entire flowsheets for all of this examples are in Chapter 7. Simulation models in this section were actually constructed by linking models for units or plant sections presented previously in this chapter (Sections 6.3 - 6.5).
6.6.1 Two turbine model simulation

The flowsheet for this model is presented in Chapter 7, Fig. 7.3 on page 153. This was a model simulated in order to provide a warm-guess for its optimisation using the filterSQP code (Chapter 7, Section 7.3). The flowsheet was taken from (Zoppke-Donaldson, 1995), where linear physical properties were used. The pump was actually modelled with the valve model (Appendix D, Section D.14). For this simulation we consider water/steam streams specific volume ‘v’. By counting equations and variables we have:

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>9 (9) = 81</td>
<td>9 (12) = 108</td>
</tr>
<tr>
<td>Steam turbines:</td>
<td>2 (8) = 16</td>
<td>2 (8) = 16</td>
</tr>
<tr>
<td>Heater/cooler:</td>
<td>2 (3) = 6</td>
<td>2 (2) = 4</td>
</tr>
<tr>
<td>Pumps (with valve model):</td>
<td>2 (3) = 6</td>
<td>2 (1) = 2</td>
</tr>
<tr>
<td>Splitters:</td>
<td>1 (5) = 5</td>
<td>0</td>
</tr>
<tr>
<td>Mixers:</td>
<td>1 (4) = 4</td>
<td>0</td>
</tr>
</tbody>
</table>

So there were (130 – 118) = 12 degrees of freedom for the whole two turbine system. From that simple consideration, the following 12 variables were fixed:

<table>
<thead>
<tr>
<th>Boiler IN-stream:</th>
<th>P</th>
<th>T</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiler OUT-stream:</td>
<td>T</td>
<td>ΔP</td>
<td></td>
</tr>
<tr>
<td>Boiler:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP turbine:</td>
<td>ηM</td>
<td>P</td>
<td></td>
</tr>
<tr>
<td>HP turbine OUT-stream:</td>
<td>ηiso</td>
<td>P</td>
<td></td>
</tr>
<tr>
<td>Splitter OUT-stream.1 = HP Turbine IN-stream:</td>
<td>F</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP Turbine OUT-stream:</td>
<td>P</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP Turbine:</td>
<td>ηM</td>
<td>ηiso</td>
<td></td>
</tr>
</tbody>
</table>

Then the EA found one redundant equation (the mass balance for the mixer) and one unspecified variable in the model. In fact the redundant mass balance equation in the ‘two turbine model’ (flowsheet in Chapter 7, Fig. 7.3 on page 153) is because this system is a ‘closed loop’, with no IN/OUT-streams. This implies that we needed to specify one additional variable. Then we have considered the fixed degrees of freedom shown in the last table and q = 1.0 (for the outlet stream of the condenser, i.e. saturated liquid, as physically required). The equation analyser then found zero free variables and one redundant equation (the one mentioned).

The starting guess considered default heat loads ‘Q’ of 5.0×10^4 kW for boiler and condenser \(^8\) and the default water/steam streams variable values given in Table 6.1 (Section 6.1). Using a TR=1.0, we solved this problem in 10 iterations.

\(^8\) actual converged values are \(Q = 30.445 \times 10^3\) kW for boiler and \(Q = -21.388 \times 10^3\) kW for the condenser.
6.6.2 Combined cycle (one pressure steam level)

This simulation was performed in order to get a starting point for the optimisation problem of a single pressure steam combined cycle (in Chapter 7, Section 7.4). This system model was constructed by linking the ‘two turbine model’ (Section 6.6.1) with a gas turbine exhaust as the source of heat (instead of a boiler of the original ‘two turbine model’). We consider here the water/steam ‘v’. For this plant the number of variables and equations are given in the following table:

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>15</td>
<td>15 (9) = 135</td>
</tr>
<tr>
<td>Steam turbines:</td>
<td>2</td>
<td>2 (8) = 16</td>
</tr>
<tr>
<td>Condenser:</td>
<td>1</td>
<td>1 (3) = 3</td>
</tr>
<tr>
<td>Pumps (with valve model):</td>
<td>2</td>
<td>2 (3) = 6</td>
</tr>
<tr>
<td>Splitters:</td>
<td>1</td>
<td>1 (5) = 5</td>
</tr>
<tr>
<td>Mixers:</td>
<td>1</td>
<td>1 (4) = 4</td>
</tr>
<tr>
<td>Exhaust gas streams:</td>
<td>3</td>
<td>3 (4) = 12</td>
</tr>
<tr>
<td>Heat recovery sections:</td>
<td>3</td>
<td>3 (14) = 42</td>
</tr>
<tr>
<td>Splitters:</td>
<td>1</td>
<td>1 (5) = 5</td>
</tr>
<tr>
<td>Steam drums:</td>
<td>1</td>
<td>1 (8) = 8</td>
</tr>
<tr>
<td>Gas turbine:</td>
<td>1</td>
<td>1 (83) = 83</td>
</tr>
<tr>
<td>Total:</td>
<td>31</td>
<td>319</td>
</tr>
</tbody>
</table>

So there were \((370 - 319) = 51\) degrees of freedom for the whole single pressure steam combined cycle.

The following fixed variables were given:

- Regarding the gas turbine, we left its fixed variables as detailed in Section 6.4.1, i.e. 26 variables.
- With respect to the HRSG, the fixed variables are (13 variables):

  - Superheater: \(\eta_{HX}, \Delta P_{hs}, \Delta P_{cs}, Ft\)
  - Evaporator: \(\eta_{HX}, \Delta P_{hs}, Ft\)
  - Economiser OUT-stream: \(T, \Delta P_{hs}, \Delta P_{cs}, Ft\)
  - Drum saturated steam IN-stream: \(q = 0.0\)
  - Economiser: \(\eta_{HX}, \Delta P_{hs}, \Delta P_{cs}, Ft\)

  Note that ‘UA’ for the heat recovery sections was not fixed, thus calculated in the simulation for the specified steam conditions.

- For the ‘two turbine model-part’ we fixed the following 12 variables:
Steam from HRSG: $F, \quad T = 400^\circ C, \quad P$

Steam to LP turbine: $F$

HP steam turbine: $\eta_M, \quad \eta_s, \quad \text{OUT-stream } P$

LP steam turbine: $\eta_M, \quad \eta_s, \quad \text{OUT-stream } P$

Cooler: $\Delta P, \quad \text{OUT-stream } q = 1.0$

The EA confirmed the appropriate definition of the model for this system finding no redundant equations nor free variables. The simulation converged in 6 iterations without the use of a TR. The initial model contained a fully converged starting guess for the gas turbine, and partially converged guesses for the rest of the system (because they were taken from the simulation of separate subsections that did not necessarily satisfy the equations in this linked model).

### 6.6.3 Combined cycle (double pressure steam level)

This model considers a double pressure steam combined cycle. It considers a steam injected gas turbine (SIGT), the production of HP steam (for power generation in steam turbines) and LP steam for deaeration purposes. The plant has an air-cooler condenser, pumps and auxiliaries. The actual flowsheet is presented in Chapter 7, Fig. 7.5 on page 165. This model has water/steam and air streams with ‘$v$’.

From the list of variables given by FMS, we have 780 variables and equations. 187 of which were fixed variables accounting for: the independent stream variables; units’ parameters; the component identification (needed for modelling gas streams multicomponents in FMS); and the number of inlet and outlet streams for mixers/splitters.

The EA confirmed the proper definition of this model by identifying zero redundant equations and zero free variables. We then solved the simulation problem (without using TR) in only 6 iterations using warm guesses for plant-sections.

### 6.6.4 A real cogeneration plant

This is a cogeneration plant currently in operation at The University of Florida, USA (Gator-Power, 1994). We simulated big plant-subsections (Sections 6.5.2 - 6.5.3) which now are assembled together in order to model and simulate the complete plant.

The whole cogeneration plant is represented in a flowsheet in Chapter 7, Fig. 7.7 on page 172.
The plant's gas turbine (a General Electric LM 6000) with steam injection produces electricity, the turbine exhaust is the source of heat for a HRSG where steam at three different pressure levels is produced. LP steam is used for deaeration purposes and for LP steam heating demands. HP steam is generated for steam injection to the gas turbine and for HP steam demand to the desuperheater # 1 (DSH # 1 in flowsheet presented in Chapter 7, Fig. 7.7 on page 172. Finally IP steam is generated for satisfying heating demands to the desuperheater # 2 (DSH # 2 in the stated flowsheet). The plant has two water/water heat exchangers that are used for preheating the condensate to be deaerated thus minimising the LP steam needed to deaerate the condensate.

The plant was simulated for providing a warm-guess for the profit optimisation problems presented in Chapter 7, Section 7.6.1 and includes the water/steam streams 'v'. We simulate (and then optimise) this plant without the assumption of supplementary firing. However, the real cogeneration plant could operate with or without supplementary firing.

For the three main sub-sections of the cogeneration plant the number of variables and equations is presented in Table 6.19. Using data from the plant sub-sections shown in Table 6.19 we obtain the number of variables and equations for the linked model of the cogeneration plant at The University of Florida (Table 6.20). In the construction of the linked plant model we should consider that there is one 'connecting' stream between the gas turbine (GT) and the HRSG (the GT exhaust) and there are also seven 'connecting' streams between the HRSG and the water/steam distribution system. These ideas are used accordingly in Table 6.20 for obtaining the total number of variables and equations for the whole plant, without double counting these streams.

So from values in Table 6.20 there are $1,275 - 1,147 = 128$ degrees of freedom. We do not give a full list of fixed variables needed for the simulation, but the next illustrative list of variable specifications:  

- the HP water flow to HP economiser number 3;
- the IP water flow to IP economiser;
- the LP water flow to LP steam drum for steam generation;
- water/water heat exchangers overall heat transfer coefficients and '$UA$';
- the steam conditions for the heating demand loads;

---

9 See also the plant flowsheet in Chapter 7, Fig. 7.7 on page 172.
- the steam losses;
- the ambient conditions;
- pumps efficiencies and pressure change;

Table 6.19: Modelling variables and equations for the main sub-sections of the real cogeneration plant.

<table>
<thead>
<tr>
<th>Steam injected gas turbine (SIGT)</th>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel-IN compressor:</td>
<td>1</td>
<td>4</td>
<td>11</td>
</tr>
<tr>
<td>Fuel compressor:</td>
<td>1</td>
<td>10</td>
<td>6</td>
</tr>
<tr>
<td>Fuel-OUT compressor:</td>
<td>1</td>
<td>4</td>
<td>11</td>
</tr>
<tr>
<td>Air-IN gas turbine compressor section:</td>
<td>1</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Gas turbine compressor section:</td>
<td>1</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>Air-OUT gas turbine compressor section:</td>
<td>1</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Steam to combustor:</td>
<td>1</td>
<td>4</td>
<td>7</td>
</tr>
<tr>
<td>Steam/Air/fuel mixer:</td>
<td>1</td>
<td>12</td>
<td>0</td>
</tr>
<tr>
<td>Combustion chamber IN-stream:</td>
<td>1</td>
<td>4</td>
<td>14</td>
</tr>
<tr>
<td>Combustion chamber:</td>
<td>1</td>
<td>16</td>
<td>14</td>
</tr>
<tr>
<td>Expansion section-IN stream:</td>
<td>1</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>Gas turbine expansion section:</td>
<td>1</td>
<td>11</td>
<td>6</td>
</tr>
<tr>
<td>Exhaust gas:</td>
<td>1</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>Power output equation:</td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Total for the sub-system:</td>
<td>14</td>
<td>89</td>
<td>117</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>HRSG</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>31</td>
<td>31 (9) = 279</td>
<td>31 (12) = 372</td>
</tr>
<tr>
<td>Gas streams:</td>
<td>12</td>
<td>12 (4) = 48</td>
<td>12 (12) = 144</td>
</tr>
<tr>
<td>Heat recovery sections:</td>
<td>11</td>
<td>11 (14) = 154</td>
<td>11 (8) = 88</td>
</tr>
<tr>
<td>Splitters:</td>
<td>4</td>
<td>4 (5) = 20</td>
<td>0</td>
</tr>
<tr>
<td>Mixers:</td>
<td>1</td>
<td>1 (4) = 4</td>
<td>0</td>
</tr>
<tr>
<td>Steam drums:</td>
<td>3</td>
<td>3 (8) = 24</td>
<td>3 (1) = 3</td>
</tr>
<tr>
<td>Valve:</td>
<td>1</td>
<td>1 (3) = 3</td>
<td>1 (1) = 1</td>
</tr>
<tr>
<td>Total for the sub-system:</td>
<td>62</td>
<td>532</td>
<td>608</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Water/steam distribution system</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/steam streams:</td>
<td>48</td>
<td>48 (9) = 432</td>
<td>48 (12) = 576</td>
</tr>
<tr>
<td>Condensing loads:</td>
<td>2</td>
<td>2 (3) = 6</td>
<td>2 (2) = 4</td>
</tr>
<tr>
<td>Mixers:</td>
<td>5</td>
<td>5 (4) = 20</td>
<td>0</td>
</tr>
<tr>
<td>Splitters:</td>
<td>9</td>
<td>9 (5) = 45</td>
<td>0</td>
</tr>
<tr>
<td>Pumps:</td>
<td>4</td>
<td>4 (8) = 32</td>
<td>4 (8) = 32</td>
</tr>
<tr>
<td>Water/water heat exchanger:</td>
<td>2</td>
<td>2 (10) = 20</td>
<td>2 (9) = 18</td>
</tr>
<tr>
<td>Valves:</td>
<td>9</td>
<td>9 (3) = 27</td>
<td>9 (1) = 9</td>
</tr>
<tr>
<td>Deaerator:</td>
<td>1</td>
<td>1 (11) = 11</td>
<td>1 (7) = 7</td>
</tr>
<tr>
<td>Total for the sub-system:</td>
<td>80</td>
<td>593</td>
<td>646</td>
</tr>
</tbody>
</table>
Table 6.20: Modelling variables and equations for the whole cogeneration plant.

<table>
<thead>
<tr>
<th>Units</th>
<th>equations</th>
<th>variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam injected gas turbine:</td>
<td>1</td>
<td>89</td>
</tr>
<tr>
<td>HRSG:</td>
<td>1</td>
<td>532 − 4 = 528</td>
</tr>
<tr>
<td>Water/steam system:</td>
<td>1</td>
<td>593 − 7(9) = 530</td>
</tr>
<tr>
<td>Total:</td>
<td>3</td>
<td>1,147</td>
</tr>
</tbody>
</table>

- water/water heat exchangers pressure drops;
- ppm of oxygen to be removed (given by the IN and OUT ppm of $O_2$ in water streams to/from the deaerator);
- deaerator operating pressure;
- gas turbine IN-streams (air and gas fuel) independent variables;
- turbomachinery and combustion efficiencies;
- the extent of reaction for unconsidered dissociation reactions in the combustor;
- the heat recovery (HR) equipment pressure drops, 'UA' and heat exchange efficiencies.

For such specifications, the EA found no redundant equations nor free variables confirming the proper model definition.

It is important to mention that for this plant simulation model FMS got 1450 modelling variables and equations, 1,275 of them are the modelling variables related to unit models (as detailed in Table 6.20) and the rest (i.e. 1,450 − 1,275 = 175) are variables for denoting component identification in gas streams and the number of streams from/to mixers/splitters that have to be fixed to fully define the model in FMS.

This problem converged using the sparse solver in 5 iterations without using TR, evidently helped by the the partial solutions from which it was started.

All the available variables in the original design that could be compared are in very good agreement with our predicted plant simulation, as shown for the decomposed problem simulations.
6.6.5 Synthesis model for a fixed structure

This model was constructed to define one of the synthesis problems (Chapter 8, Section 8.3), which involves the optimal synthesis of heat recovery (HR) coils within a double pressure steam combined cycle. The corresponding flowsheet is presented in Chapter 7, Fig. 7.8, on page 180, where we also solved this model using the filterSQP optimisation code. The plant model has a LM 6000 gas turbine (Section 6.4.1), the hyperstructure defined in Chapter 3, Section 3.5.3 and a steam system which is part of the combined cycle described in Section 6.6.3.

For obvious reasons a warm-starting point for a synthesis problem is very difficult (or even impossible) to obtain by simulation, since we do not know what the optimal structure looks like. Nevertheless, the simulation of this model for a fixed structure was deemed necessary in order to assess the correctness of model definition and to provide a 'sensible' starting point for the solution of the synthesis problem. Afterwards, further to the successful simulation of a fixed structure, we then freed some variables to solve the synthesis model. To construct this complex model in FMS we use several submodels which were then linked (see Fig. 8.4 on page 200 in Chapter 8).

In order to perform this simulation we assumed a fixed structure from the model to be used for synthesis. We assume the 8 HR exchangers operating in series with respect to the hot side stream. This means that gas turbine exhaust goes through each of the HP superheaters, then goes to the HP evaporator, then through each of the HP economisers and finally passes to the LP evaporator. As mentioned in Chapter 3, Section 3.5.3, the hyperstructure involves splitters/mixers for the hot/cold side in HR equipments, e.g. the exhaust gas from the gas turbine should be 'split' in 8 streams going to each of the HR exchangers.

For large-scale problems of these dimensions, our initial procedure of 'hand made counting' of variables and equations is impractical. We therefore defined this model in FMS using tested plant sections where available. The model resulted with 3,022 variables and equations. FMS spent about 4 minutes in the initialisation of this model in our Sparc 2 workstation.

For the successful simulation we fixed the following variables: 10

- all the integer variables for HR exchangers (z=1);
- all the independent mass flows to/from mixers/splitters defining the hyperstructure (they

10 See also flowsheet in Fig. 7.8, on page 180.
are 79 and consider all HR equipments in series as explained above):

- 7 OUT-stream flows from gas turbine splitters: 6 of them equal to $1.0 \times 10^{-7}$ (our 'zero' value for exhaust gas streams) and one molar flow having the gas turbine exhaust total flow minus $6.0 \times 10^{-7}$. As explained before, the gas turbine splitters have 1 IN and 8-OUT streams. Since there are nine of such splitters in the superstructure then we have 63 fixed variables;

- 2 OUT-stream flows from water/steam splitters (defining the 'cold side' superstructure): one mass flow fixed to $F = 6.6 \text{ kg/s}$ (passing through HR exchangers) and another mass flow fixed to 0.0 kg/s. Here we have a total of 16 fixed variables.

  - 'T' of deaerated water, 'P' in Deaerator;

  - the HP water mass flow for the HP steam system;

  - OUT-stream 'T' from the 3 HP superheaters and from HP economisers 2 and 3.

  - HP steam drum $\Delta T_{Drum}$ (defines the preheating 'T' of water to the steam drum since is the difference between $T_s$, the saturation temperature and the stream 'T');

  - HP and LP steam drums blow down;

  - the gas turbine independent variables (specified in Section 6.4.1).

  - OUT-stream 'P' from steam turbines. Also flow to LP steam turbine;

  - the HR exchangers' independent variables (as in the hyperstructure simulation shown in Section 6.5.5).

After fixing the stated specifications the EA found zero free variables and 81 redundant equations. All of them are momentum balances around mixers/splitters defining the hyperstructure and the pressure drop equations for HR (in the hot side and in the cold side) for which we specified $\Delta P = 0$.

This identification of free variables and redundant equations was performed in EA stage (1): structural analysis. Then the EA did stage (2): numerical analysis and spent about 40 minutes creating a huge file while performing "swapping columns" and an enormous amount of 'fill-in' (Morton and Collingwood, 1998). We believe performance of the EA can be improved (for large-scale problems) by having the option for the user to perform only stage (1) to report free variables and redundant equations. Almost certainly we are learning nothing about model
validity from stage (2) and all we are seeing is an effort to get around numerical singularities caused by the default guesses.

The starting guess for this large-scale model considers:

- Converged values from the gas turbine exhaust (at this equipment nominal capacity) for all mixers defining the hot-side superstructure. The gas turbine exhaust has $T = 473°C$.
- Converged values for the steam system-part.
- For gas turbine splitters defining the hot-side superstructure: converged values for gas turbine exhaust at the gas turbine outlet minus 100.0 °C.
- For water/steam mixers/splitters in cold-side superstructure: use liquid, saturated or superheated converged stream variables values for relevant streams.
- Note that although converged partial solutions were used, they did not necessarily 'match' at process streams inter-connections.
- Slack variables all have been initialised as 1.0 except the ones related to Heat loads $Q$ which are $1.0 \times 10^3$.

Finally, the whole synthesis model for a given fixed structure was simulated in 7 iterations of the NLAE solver without the use of TR. The NLAE solver spent about 15 seconds per iteration (the first iteration took longer, i.e. about 3 minutes which were taken by the solver for reordering equations).

The independent flows in hot side superstructure that cannot be specified as exactly zero\(^{11}\) (but as $1.0 \times 10^{-7}$ kmol/s) produced temperature changes (in relevant mixers) of about 0.01°C only. Thus the exhaust temperature profile is well calculated for the hot side superstructure considering our 'zero' molar flow for exhaust gas streams.

Note also that the zero flow for some of the water/steam streams defining our fixed structure for the synthesis model did not cause any convergence problems for this simulation.

\(^{11}\) to avoid numerical problems with mole balance equations for gas streams.
6.7 Performance of software and models for EO simulation

After the many experiments shown on solving simulation problems by simultaneous equations, in this section we present an overview of the performance of software and models for EO simulation of utility systems. As mentioned, converged simulations provide the strategy for giving warm starting guesses for the robust solution of NLP optimisation problems presented in Chapter 7.

6.7.1 Performance of the modelling system (FMS)

To model simulation problems from simple entities, complex units, plant sections up to complete combined heat and power (CHP) systems, we have taken advantage of the many capabilities of the modelling system FMS.

By constructing models of up to around 3,000 variables and equations we have shown that large-scale models in CHP (and potentially in general Process Systems Engineering) can easily be built with FMS.

We have found no restriction from FMS to construct our plant models, using individual entities, complex units and plant sections to build together whole industrial scale combined heat and power systems. For the largest model (more than 3,000 variables) FMS spends about 4 minutes in setting up the model in a Sparc 2 workstation.

The capability of FMS to interface with several software packages for equation-based simulation, optimisation and synthesis made this system a very useful environment for a simultaneous approach.

6.7.2 Performance of the equation analyser (EA)

We tested the EA performance under a large number of different and complex problems from small to large-scale.

It is important to use the EA for models to be optimised/simulated. In these experiences we found the EA to be highly reliable for the identification of the number of free variables and for
pointing to the redundant equations in a given model.

The identification of free variables and redundant equations in the EA is done in two stages: (1) performing *symbolic or structural analysis*, resulting in an 'output assignment' (Morton and Collingwood, 1998) to identify redundant equations and free variables. This is a relatively fast action. However, *numerical analysis* (stage (2) in the EA) may require "swapping columns" to try and find pivots for Gaussian elimination of the Jacobian. This produces huge files for large-scale problems (with more than 3,000 variables) and takes a long time (about 40 minutes). Stage (2) in the EA is designed to spot numerical dependency in equations. However, in large-scale nonlinear systems most numerical singularities are due to the starting guess. Genuine numerical dependencies between equations are hard to spot.

It may be desirable to have the option from the EA to perform only stage 1 (*structural analysis*) especially for large-scale models, and in any case to avoid the creation of large files, even if Gaussian elimination is performed.

For all the problems analysed with the EA we found that, using the default parameters e.g. matrix blocking (Morton and Collingwood, 1998) the EA is very robust and fast for problems up to around 1,500 variables. For the analysis of larger problems (more than 3,000 variables) we used the following parameters from the EA: 12

| Equation reordering method: (Reorder equations by initial rank) | 2 |
| Block finding method: none | 1 |
| Gauss elimination method: Output variables as pivots | 1 |
| Element scaling method: With variable scaling | 3 |

Finally, we found that the EA detects very efficiently the number of free variables and redundant equations. However, for large-scale models a useful suggestion (in a simulation sense) of actual free variables to be fixed, was not always done. This is because of the following aspects of the EA:

- The user should define modelling equations in the form,

\[ OUTPUTS - INPUTS = 0 \]

- in defining our actual modelling equations for every single unit we were not strict on

---

12 This is not a complete list of the various options available in the EA, which can be found in (Morton and Collingwood, 1998).
defining our equations in such a way, e.g. some may be

\[ \text{INPUTS} - \text{OUTPUTS} = 0 \]

A strict 'form' of modelling equations can always be done when defining new models. However, a further issue for researching would be to check that models so defined will always permit the EA to accurately suggest free variables to fix, especially for the multiple-recycle hyperstructure in MINLP synthesis models.

6.7.3 Performance of the sparse NLAE solver

In all these simulations the Newton-like sparse NLAE solver proved to be robust and reliable. Quadratic convergence was observed for all the simulation examples.

From the computational experiments presented in this paper it was observed that the Newton-like sparse NLAE solver:

- Is able to solve complex problems like the one arising from the gas turbine combustor simulation (Section 6.3.5). This solution succeeded from a poor starting guess only with the use of a TR, for which initial size of 1.0 was given. This model includes equations which describe combustion and equilibrium relationships for dissociation reactions at high temperatures, along with the rest of performance and balance equations. Thus it is a difficult problem to converge with traditional NLAE solvers.

- Did not require the use of a TR for the majority of the problems solved, including some non-trivial simulations (e.g. for sub-sections of the HRSG unit in Section 6.4.2).

- Was reliable, fast and robust when solving problems of up to around 3,000 variables and equations.

- From this experience we believe that the NLAE solver can efficiently solve very large-scale simulation problems (with many thousands of variables) which may be rapidly proposed for larger CHP systems or for other engineering problems modelled in FMS.

- The computation times were in all cases around a few seconds, except for the largest model (having more than 3,000 variables), where the NLAE solver took about 300 seconds using a Sparc 2 workstation. 13

13 The NLAE solver does not report computation time, and for the largest problem it was 'wall-clock' estimated.
The solver is able to solve systems with no free variables, but some redundant equations (e.g. resulting from multiple-recycle hyperstructure models).

6.7.4 Performance of the proposed EO models

Individual streams and unit operations models were widely tested and predictions agreed very well with published data where available (e.g. (Smith and Van Ness, 1987), (Irvine and Liley, 1984), (NEL and IChemE, 1981)).

We found that the proposed equation-based models for combined heat and power systems are reliable for solving industrial scale problems. We tested the models’ predictions by comparing its results with data from the simulation of a commercial gas turbine (de Biasi, 1990) and from a cogeneration plant currently in operation (Gator-Power, 1994). For the commercial gas turbine (Section 6.4.1) models’ predictions were under 1% error compared to nominal data. For the gas turbine and HRSG (Section 6.5.2) in the real cogeneration plant all variables were predicted within 1% error, except individual heat exchangers’ loads which we predicted under 4.3% error.

Our large set of models proposed from a combination of rigorous and realistic considerations (using current design practice) performed very well in the solution of simulation problems for CHP systems.

An important aspect of convergence of models was the water/steam mass flow specified exactly equal to 0. We found that, e.g. for a valve (in flowsheet shown in Section 6.5.4), the specification of \( F = 0 \) did not allow the solution of the equations defining this unit model. That is because the energy balance \( (F_1 h_1 - F_2 h_2 = 0) \) cannot solve for the outlet enthalpy \( h_2 \), so the OUT-stream ‘\( T \)’ could not be calculated. Using a sensible ‘close-to-zero’ lower bound for water/steam streams \((1.0 \times 10^{-8} \text{ kg/s})\), allowed convergence without any problem and still sensible results.

In the simulation of a fixed structure for the MINLP synthesis model (Section 6.6.5) we have water/steam mass flow specifications of \( F = 0 \) in the superstructure model, the simulation could be done without any problem. This is because there are no valve models in the superstructure which may produce the stated problem for specified \( F = 0 \).

Fully testing and demonstration of the applicability of the proposed models was presented in this chapter.
6.8 Summary of equation-based simulation problems

In Table 6.21 we present an overview of all the simulation problems included in this chapter. For each problem we give the number of variables and equations, the number of iterations from the sparse NLAE solver for convergence and the corresponding section in this chapter where each problem was presented.

<table>
<thead>
<tr>
<th>Problem description</th>
<th>variables and equations</th>
<th>iterations</th>
<th>Section in this chapter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Individual process streams:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Water/steam stream</td>
<td>11</td>
<td>up to 13</td>
<td>6.2.1</td>
</tr>
<tr>
<td>- Multicomponent gas stream</td>
<td>11</td>
<td>3</td>
<td>6.2.2</td>
</tr>
<tr>
<td>Single units:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Steam turbine</td>
<td>30</td>
<td>11</td>
<td>6.3.1</td>
</tr>
<tr>
<td>- Compression section of a gas turbine</td>
<td>22</td>
<td>6</td>
<td>6.3.2</td>
</tr>
<tr>
<td>- Compressor for gas fuel</td>
<td>28</td>
<td>7</td>
<td>6.3.3</td>
</tr>
<tr>
<td>- Gas turbine combustor premixer</td>
<td>32</td>
<td>7</td>
<td>6.3.4</td>
</tr>
<tr>
<td>- Gas turbine combustion reaction section</td>
<td>32</td>
<td>10</td>
<td>6.3.5</td>
</tr>
<tr>
<td>- Expansion section of a gas turbine</td>
<td>30</td>
<td>6</td>
<td>6.3.6</td>
</tr>
<tr>
<td>- HP steam superheater</td>
<td>54</td>
<td>10</td>
<td>6.3.7</td>
</tr>
<tr>
<td>- Heat recovery exchanger (for MINLP model)</td>
<td>82</td>
<td>9</td>
<td>6.3.8</td>
</tr>
<tr>
<td>- Multicomponent gas streams mixer/splitter:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Combustor premixer for a SIGT</td>
<td>40</td>
<td>6</td>
<td>6.3.9</td>
</tr>
<tr>
<td>- Steam/fuel/air splitter</td>
<td>56</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>- Gas turbine exhaust splitter with 8 OUT-streams</td>
<td>173</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>Complex unit operations:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- A commercial gas turbine</td>
<td>109</td>
<td>32</td>
<td>6.4.1</td>
</tr>
<tr>
<td>- HRSG (subsection simulation):</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- HP steam superheaters and HP evaporator</td>
<td>214</td>
<td>12</td>
<td>6.4.2</td>
</tr>
<tr>
<td>- IP superheater, HP economisers 1 and 2 and IP evaporator</td>
<td>203</td>
<td>21</td>
<td></td>
</tr>
<tr>
<td>- LP Steam drum and LP evaporator</td>
<td>99</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>- IP economiser and HP economiser 3</td>
<td>96</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>- HRSG (complete unit)</td>
<td>543</td>
<td>42</td>
<td>6.4.3</td>
</tr>
<tr>
<td>Plant sections:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Air compression system</td>
<td>48</td>
<td>7</td>
<td>6.5.1</td>
</tr>
<tr>
<td>- Gas turbine and HRSG</td>
<td>648</td>
<td>25</td>
<td>6.5.2</td>
</tr>
<tr>
<td>- Water/steam distribution system</td>
<td>594</td>
<td>15</td>
<td>6.5.3</td>
</tr>
<tr>
<td>- Rankine cycle-part of a combined cycle</td>
<td>447</td>
<td>9</td>
<td>6.5.4</td>
</tr>
<tr>
<td>- Hyperstructure for the synthesis of HP steam superheaters</td>
<td>514</td>
<td>7</td>
<td>6.5.5</td>
</tr>
<tr>
<td>Whole utility systems:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Two turbine model</td>
<td>130</td>
<td>10</td>
<td>6.6.1</td>
</tr>
<tr>
<td>- Combined cycle (one pressure steam level)</td>
<td>370</td>
<td>6</td>
<td>6.6.2</td>
</tr>
<tr>
<td>- Combined cycle (double pressure steam level)</td>
<td>780</td>
<td>6</td>
<td>6.6.3</td>
</tr>
<tr>
<td>- A real cogeneration plant</td>
<td>1,450</td>
<td>5</td>
<td>6.6.4</td>
</tr>
<tr>
<td>- Synthesis model for a fixed structure</td>
<td>3,022</td>
<td>7</td>
<td>6.6.5</td>
</tr>
</tbody>
</table>
Chapter 7

Optimisation results and discussion

This chapter presents the NLP optimisation problems solved in utility systems. Problems size range from 130 to more than 3,000. These computational experiments were done on a Sparc 2 workstation and are described below.

Since we have proposed and implemented equation based models for these systems, the following two initial stages were done:

- Testing the performance of the proposed equation oriented models for solving utility optimisation problems. To do this we used the 'tolerance-tube' SQP method described in Chapter 4, Section 4.2.1 to solve a problem for a Heat and Power System with steam turbines and air compressors (Section 7.1).

- Experimenting on the 'two turbine model' (Section 7.3). In order to test the filterSQP optimisation code interfaced to our modelling system FMS, we solved a number of examples for this model.

After that, using the filterSQP code and FMS, we solved a number of thermal efficiency and economic optimisation problems for complex systems (including profit optimisation problems for a real cogeneration plant). Results of these problems are presented in Sections 7.4 - 7.7. In solving the optimisation examples we used a 'warm' starting point, obtained by solving a fully converged simulation problem as explained in Chapter 6. We use a filterSQP solver tolerance of $1.0 \times 10^{-6}$ for the solution of all the optimisation problems in this chapter.
For each optimisation example we give: a brief problem statement; the flowsheet representing the system; results produced from the SQP optimisation package; and, an analysis of the optimised variables and objective function. The optimised objective function is this chapter is referred to as $f(x^*)$.

The problem solved with the ‘tolerance-tube’ SQP method (Section 7.1) does not consider the specific volume ‘$v$’ calculation in air and water/steam streams, while in the rest of the optimisation problems we consider the calculation of ‘$v$’ for these streams.

The performance of the filterSQP optimisation code is discussed in Section 7.8. A summary of the problems solved in this chapter is presented in Section 7.9, where we provide a table showing a description of all the optimisation problems, including the total number of variables and equations, the number of degrees of freedom and fixed specifications as well as the number of iterations needed for their solution.

7.1 Heat and power system with steam turbines and air compressors

To solve this optimisation problem we used the ‘tolerance-tube’ SQP method (described in Chapter 4, Section 4.2.1). This SQP code was used in the early stages of this project, when we initially tested the proposed models and did not use FMS.

This Heat and Power System has been described in (Morton, 1994b) and is referred to as the “MASSBAL” problem. As illustrated in Fig. 7.1, steam at 4.24 MPa (identified in Fig. 7.1 as 600#.HEADER) is produced in a steam generator.

The system supplies steam at three pressure levels. The steam turbines are connected either to electric generators or air compressors. There are two condensing turbines. The plant total electricity and compressed air demands, which are specified, are completed by purchased power and by using reciprocating air compressors driven by purchased power. The air system consists of two sets of compressors:

- turbocompressors (marked $TC.COMP$ in Fig. 7.2), for which the power input is the sum of the outputs from the turbines $TC3$ and $TC4$, see Fig. 7.1;
- reciprocating compressors (marked $RECIP.COMP$ in Fig. 7.2), which are driven by
using purchased electricity.

As shown in Fig. 7.1 the extractions from interstage steam turbines are collected in headers at lower pressure levels: 1.14 MPa and 0.45 MPa (identified in Fig. 7.1 as 150#.HEADER and 50#.HEADER respectively).

Figure 7.1: The steam system in the MASSBAL problem.
Additional restrictions

- The compressed air demand is 5.9 m$^3$/s, expressed by:

$$v_a F - 5.9 = 0.0$$ (7.1)

- The pressure of the air supplied by the compressors should be 0.515 MPa.

- The split ratio of air through the parallel compressors in Fig. 7.2 is decided by the power given by the turbocompressor, \((TC.COMP)\) in Fig. 7.2, which is related to the power available from the turbocompressor \(TC\) turbine stages in Fig. 7.1 by:

$$\text{(TC.COMP)}_{power} = (TC3)_{power} + (TC4)_{power}$$ (7.2)

- Power system performance specifications: each turbogenerator (TG1 - TG3) has a total power defined as the sum of its stage power outputs. The total plant power demand plus the reciprocating air compressor power demand equals the sum of purchased and cogenerated power.

All turbine stages have fixed mechanical and isentropic efficiencies (Morton, 1994b).

The optimisation problem

In this problem we want to find the optimum steam mass flows through the 9 turbine stages as well as the mass flow through the ‘600.LETDOWN’ valve (see Fig. 7.1), that is 10 free variables.
The economic objective function, 'O.F.' in \( \$/s \) consists of minimising the cost of purchased electricity and steam generation given by:

\[
O.F. = \text{Purchased power cost} + \text{Steam generation cost}
\]  

(7.3)

where,

\[
\begin{align*}
\text{Purchased power cost} &= \left(2.22 \times 10^{-5} \ \$/kJ\right) \left(\text{purchased power, kW}\right) \\
\text{Steam generation cost} &= \left(6.6 \times 10^{-3} \ \$/kg \text{ HP steam}\right) \left(\text{HP steam flow, kg/s}\right)
\end{align*}
\]

These data cost are only used for the "MASSBAL" problem (Morton, 1994b). The rest of the optimisation problems in this chapter use economic data from Appendix E.

The constraints for this optimisation problem consist of the modelling equations for:

- the 34 water/steam streams involved,
- the 9 stage steam turbines,
- the 8 mixers-splitters in the steam system,
- the 2 let-down valves,
- the two steam condensers,
- the 6 air streams in the air system,
- the 2 mixers-splitters in the air system,
- the 2 air compressors,
- the compressed air demand,
- the split flow of air through the parallel compressors,
- the power system performance specifications

and lower and upper bounds on all system variables. Specifications are supplied as equal upper and lower bounds on the fixed variables.

For this problem, the optimum solution as well as some characteristics of the system are described in Table 7.1. The optimum solution gave the optimum value for our 10 decision variables: 9 steam mass flows through the turbine stages as well as the mass flow through the
600.LETDOWN valve (see Fig. 7.1). The solution for the remaining 456 modelling variables from the same number of equations (see Table 7.1) is obtained at the same time. Values for the 10 optimised mass flow are given in Table 7.2.

This model is somewhat too large to be tackled conveniently by traditional SQP techniques which use dense Jacobian and approximate Hessian matrices, the latter being updated after each QP by a BFGS algorithm or similar (Fletcher, 1987). This example demonstrates the successful performance of our proposed models (tested in the early stages of this research) and ability of the tolerance-tube SQP code to solve successfully a medium size utility optimisation problem which is non-trivial and contains substantial nonlinearity.

The ‘tolerance-tube’ SQP method was, in our experience, very robust. However, further developments in SQP methods from researchers at Dundee University, produced an advanced package called filterSQP. So we decided to use the newest method for the rest of this research.

<table>
<thead>
<tr>
<th>Table 7.1: Optimisation results. MASSBAL problem.</th>
</tr>
</thead>
<tbody>
<tr>
<td>*<em>Final value f(x</em>), [$/s]**: 0.2958</td>
</tr>
<tr>
<td><strong>Iterations</strong>: 54</td>
</tr>
<tr>
<td><strong>Total CPU time (s)</strong>: 342.6</td>
</tr>
<tr>
<td><strong>Cogenerated power, [kW]</strong>: 12,030</td>
</tr>
<tr>
<td><strong>Purchased Power, [kW]</strong>: 1,220</td>
</tr>
<tr>
<td><strong>variables</strong>: 500</td>
</tr>
<tr>
<td><strong>equations</strong>: 456</td>
</tr>
<tr>
<td><strong>specifications</strong>: 34</td>
</tr>
<tr>
<td><strong>free variables</strong>: 10</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stream</th>
<th>starting value</th>
<th>optimised value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TG1.HP.SECT IN-stream:</td>
<td>3.75</td>
<td>3.8794</td>
</tr>
<tr>
<td>TG1.LP.SECT IN-stream:</td>
<td>2.00</td>
<td>3.8794</td>
</tr>
<tr>
<td>TG2 IN-stream:</td>
<td>5.94</td>
<td>6.9239</td>
</tr>
<tr>
<td>TG3.HP.SECT IN-stream:</td>
<td>13.75</td>
<td>13.076</td>
</tr>
<tr>
<td>TG3.MP.SECT IN-stream:</td>
<td>7.00</td>
<td>11.250</td>
</tr>
<tr>
<td>TG3.LP.SECT IN-stream:</td>
<td>4.00</td>
<td>11.250</td>
</tr>
<tr>
<td>TC3 IN-stream:</td>
<td>3.75</td>
<td>6.2500</td>
</tr>
<tr>
<td>TC4.HP.SECT IN-stream:</td>
<td>4.38</td>
<td>7.5000</td>
</tr>
<tr>
<td>TC4.LP.SECT IN-stream:</td>
<td>2.00</td>
<td>4.3261</td>
</tr>
<tr>
<td>600.LETDOWN IN-stream:</td>
<td>3.12</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
7.2 Results reported from the filterSQP for optimised models

In this section we briefly explain the type of results reported from the filterSQP code for the optimised models in Sections 7.3 - 7.7. For a given optimisation model, we ran the filterSQP solver then it reports convergence parameters and finally, we could look at the optimised variable values (using the modelling system FMS). So the parameters reported by filterSQP and presented for each optimised model are:

- the CPU time (s); the number of iterations (and how many of them were infeasible NLPs);
- the number of quadratic programming (QP) problems solved (equal to the number of Hessian evaluations);
- the total number of QP pivots. This is the number of times, in solving QPs, that a column is pivoted;
- the number of function, constraint and gradient evaluations;
- the optimised objective function $f(x^*)$; the initial/final trust region (TR) size;
- the dimension of null space, given by the number of variables less the number of active constraints at solution (equations + active bounds).

In all our optimisation problems we observed values for the dimension of null space (dns) of 0 and 1. 'dns=0' implies a solution 'lying in a corner' i.e. like in linear programming where an optimum lies at a fully constrained vertex of the constraints. 'dns=1' implies that at solution there is one variable which could be independently varied while not changing the active set.

It should be also mentioned that we use two versions of the filterSQP code. We use the dense version for solving problems in Section 7.3.1, where the effect of scaling is presented. Dense and sparse versions are different in the relevant format for specifying QP problems and in the matrix algebra modules.

In Sections 7.3.2 and 7.5.2 we compare the performance of dense vs. sparse versions for solving problems of different size and complexity. All other optimisation problems in this chapter were solved with the sparse version.
All economic optimisation problems solved with the filterSQP code consider capital and operating costs based in 1997 prices as explained in Chapter 3, Section 3.4.2 and in Appendix E.

### 7.3 Two turbine model optimisation

Optimisation problems in this section and the rest of this chapter use the filterSQP code (Fletcher and Leyffer, 1998), an advanced NLP optimisation method with a ‘filter’ to promote global convergence. They use also the modelling system FMS and contain water/steam and air streams specific volume \((v)\) as stream variable.

The ‘two turbine model’ represents a two-stage Rankine cycle with regenerative feed heating and is illustrated in Fig. 7.3. Steam is generated at high pressure and temperature and passed through a steam turbine, part of whose exhaust is used to raise the energy of returned feed water from the low pressure section. The low pressure (LP) turbine uses the rest of the high

![Figure 7.3: Two turbine model.](image-url)
pressure (HP) turbine exhaust and its partially condensed exhaust is then fully condensed in a heat exchanger. The condensate is pumped in two stages to the boiler. A constraint on the bleed steam from the HP turbine is that the fluid entering the HP pump must contain no vapour \((q > 1)\).

The optimisation problem consisted in maximising the thermal efficiency of the plant subject to specified flow rate (10 kg/s in the HP section), boiler outlet temperature and pressure (550 °C and 2.0 MPa respectively), and turbine efficiencies (0.95 and 0.8 for mechanical and isentropic efficiencies respectively). We also fixed pressure drops through ‘boiler’ and ‘cooler’ (see Fig. 7.3) to be 0. The condensate temperature has a lower bound (taken as 50 °C) and this stream must be fully condensed \((q > 1)\). We have 4 free variables: OUT-stream pressure from steam turbines; steam flow to LP turbine and ‘cooler’ heat load (or outlet temperature). This problem has 130 variables, 118 constraints, 9 specifications and 4 free variables. Recall that this problem may have a maximum of 13 free variables, since it has a redundant mass balance equation produced by the closed loop (as explained in Chapter 6, Section 6.6.1) where we solved the simulation problem for this system.

The objective function is given by the plant thermal efficiency \((\eta_{th})\):

\[
\eta_{th} = \frac{W_1 + W_2}{Q_{boiler}}
\]

(7.4)

where \(W_i\) is the turbine power output \((i = 1, 2)\), and \(Q_{boiler}\) is the boiler heat load.

This is a relatively small, but not trivial problem since in our EO optimisation the constraints are highly nonlinear resulting from the accurate thermodynamic and process stream models.

A number of experiments on the solution of this problem are presented in Sections 7.3.1 - 7.3.4. We do not provide optimised variable values for each of those problems. Instead in Table 7.3 we give values for the 4 decision variables found in the solution of the TR size examples (which got all the same solution independently of initial TR values, as shown in Section 7.3.3). As can

<table>
<thead>
<tr>
<th>Table 7.3: Optimisation results. Two turbine model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final value (f(x^*)), %:</td>
</tr>
<tr>
<td>HP turbine OUT-stream (P), [MPa]:</td>
</tr>
<tr>
<td>LP turbine OUT-stream (P), [MPa]:</td>
</tr>
<tr>
<td>LP turbine IN-stream (F), [kg/s]:</td>
</tr>
<tr>
<td>Cooler heat load (Q), [kW]:</td>
</tr>
<tr>
<td>(OUT-stream at (T) lower bound i.e. 50 °C)</td>
</tr>
</tbody>
</table>
be observed, the optimum thermal efficiency is not particularly high (i.e. 28.26%). This is a function of the steam superheating temperature and the condensed temperature lower bound specified.

7.3.1 Effect of scaling example

We are aware that, since in a typical utility system optimisation problem the variables are all of very different orders of magnitude, the filterSQP solver could be inefficient due to the fact that the trust region does not discriminate between variables of different magnitudes. Nevertheless, we investigated how 'inefficient' the solver is when no scaling is used in a problem that we already knew needed to be scaled for efficient solution through a trust region SQP algorithm.

Using the filterSQP dense version with an initial trust region of 0.1 the 'two turbine model' was solved without scaling and using scaling. The scaling procedure is described in Chapter 5, Section 5.5. Results for the 'effect of scaling example' are compared in Table 7.4. As can be observed from that table, not using scaling for this problem requires more than 10 times the number of iterations compared with the case when scaling was considered. Also the number of QP pivots is substantially smaller when scaling is used. Apart from this problem all others presented in this chapter are fully scaled.

Table 7.4: Two turbine model optimisation (effect of scaling example).

<table>
<thead>
<tr>
<th>model:</th>
<th>unscaled</th>
<th>scaled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>119.6</td>
<td>31.04</td>
</tr>
<tr>
<td>Iterations:</td>
<td>104</td>
<td>10</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>57</td>
<td>6</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>193</td>
<td>18</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>11,271</td>
<td>1,234</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>125</td>
<td>6</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>194</td>
<td>20</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>50</td>
<td>11</td>
</tr>
<tr>
<td>Final value f(x*):</td>
<td>28.19 %</td>
<td>28.22 %</td>
</tr>
<tr>
<td>Initial/Final trust region size</td>
<td>0.1/3.906× 10^{-2}</td>
<td>0.1/1.6</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>
7.3.2 Dense vs. sparse filterSQP versions example

The 'two turbine model' applying scaling and an initial trust region of 0.1 was solved using both the dense and the sparse filterSQP versions. The results are shown in Table 7.5. Using the sparse version results in one iteration less than when using the dense SQP version and in about one third of the computation time for solving this problem along with almost 10 times fewer QP pivots. This is a small problem (less than 150 variables) that still could be tackled using the dense version, and no great advantage is gained from using the sparse version. Nevertheless, the advantage of using a sparse version over a dense one is still apparent. Savings in computation time and reduced data storage requirements when using the sparse version become very important when large models are optimised.

<table>
<thead>
<tr>
<th>filterSQP version:</th>
<th>dense</th>
<th>sparse</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>31.04</td>
<td>13.4</td>
</tr>
<tr>
<td>Iterations:</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>18</td>
<td>13</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>1,234</td>
<td>128</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>6</td>
<td>9</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>20</td>
<td>12</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>11</td>
<td>10</td>
</tr>
<tr>
<td>Final value f(x*):</td>
<td>28.22 %</td>
<td>28.2695 %</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>0.1/1.6</td>
<td>0.1/1.6</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

7.3.3 Initial trust region size effect example

The next set of examples shows the effect of the initial trust region 'TR' size which according to (Fletcher and Leyffer, 1998) should not affect the optimiser's ability to converge. Several experiments on the optimisation of the 'two turbine model' using different initial trust region size were done, the following set of initial TR values were used:

0.01, 0.1, 1.0, 10.0, 20.0, 100.0, 1000.0

A summary of these numerical experiments produced the results shown in Table 7.6. From this table it is observed for the TR values of 0.01 and 0.1 the numbers of iterations were 12 and 9 respectively, which are substantially higher than the number of iterations required if the initial
TR is 1.0 or greater. The use of TR=1.0 allows the solver to converge the problem in only 5 iterations with 97 QP pivots (the smallest value).

It should be mentioned (although only shown for TR=10.0 and TR=100.0 in Table 7.6) that for TR=10.0 and higher filterSQP spends only 5 iterations and got all the same solution parameters (objective function, variable values, number of QP pivots, etc.). In addition the initial and the final TR values (at convergence) were the same for all initial TR values of 10.0 and higher.

It was thus shown that filterSQP runs successfully for any TR value, the best initial values for this particular problem being TR=1.0 or higher.

The use of TR=1.0 is intuitively sensible, since it allows a move up to the scale factor magnitude in each variable.

Table 7.6: Two turbine model optimisation (initial trust region size effect example).

<table>
<thead>
<tr>
<th>Initial trust region:</th>
<th>0.01</th>
<th>0.1</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>1.42</td>
<td>1.07</td>
<td>0.54</td>
</tr>
<tr>
<td>Iterations:</td>
<td>12</td>
<td>9</td>
<td>5</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>7</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>16</td>
<td>13</td>
<td>6</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>162</td>
<td>128</td>
<td>97</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>9</td>
<td>9</td>
<td>6</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>15</td>
<td>12</td>
<td>7</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>13</td>
<td>10</td>
<td>7</td>
</tr>
<tr>
<td>Final value f(x*):</td>
<td>28.2695 %</td>
<td>28.2695 %</td>
<td>28.2695 %</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>0.01/2.56</td>
<td>0.1/1.6</td>
<td>1.0/4.0</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

| Initial trust region (cont.): | 10.0 | 100.0 |
| Total CPU time (s):           | 0.58 | 0.54  |
| Iterations:                   | 5    | 5     |
| ... of which iterations in inf. NLP: | 0    | 0    |
| QP problems solved:           | 6    | 6     |
| Total number of QP pivots:    | 99   | 99    |
| Function evaluations:         | 6    | 6     |
| Constraint evaluations:       | 7    | 7     |
| Gradient evaluations:         | 7    | 7     |
| Final value f(x*), %:         | 28.2695 | 28.2695 |
| Initial/final TR size:        | 10.0/10.0 | 100.0/100.0 |
| Dimension of null space:      | 1    | 1     |
7.3.4 Shadow price example

In the ‘two turbine model’ already described the HP steam temperature was fixed at \( T = 550^\circ C \). Here two more optimisation problems were solved by setting \( T=551^\circ C \) and \( T= 549^\circ C \) for the superheated steam, to show the ‘shadow price’ effect and to assess the performance of the model and the SQP solver.

The Lagrange Multiplier value for a given constraint indicates how much the objective function will change for a unit change in the constraint constant, if the problem is linear over the change interval. The Lagrange Multipliers are termed ‘shadow prices’ of the constraints because the change in the optimal value of the objective function per unit increase in a constant equality constraint is given by the Lagrange multiplier (Edgar and Himmelblau, 1989).

The ‘shadow price’ gives a change in the objective function as,

\[
\delta f = \nabla f \cdot \delta x = \lambda \nabla c \cdot \delta x = \lambda \delta c
\]

In this optimisation example, it was decided to modify the HP steam temperature ± 1.0 °C and in each case the optimisation problem was solved using the sparse filterSQP version. The corresponding results with initial/final trust region of 1.0/4.0 respectively are shown in Table 7.7.

<table>
<thead>
<tr>
<th>HP steam ( T, ^\circ C ):</th>
<th>550.0</th>
<th>551.0</th>
<th>549.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>5.9</td>
<td>6.7</td>
<td>6.8</td>
</tr>
<tr>
<td>Iterations:</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>QP problems solved:</td>
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<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>97</td>
<td>97</td>
<td>97</td>
</tr>
<tr>
<td>Function evaluations:</td>
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<td>6</td>
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<tr>
<td>Constraint evaluations:</td>
<td>7</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>7</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Final value ( f(x^*) ), %:</td>
<td>28.2695</td>
<td>28.2867</td>
<td>28.2524</td>
</tr>
<tr>
<td>(or, for the optimiser):</td>
<td>-0.282695</td>
<td>-0.282867</td>
<td>-0.282524</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>1.0/4.0</td>
<td>1.0/4.0</td>
<td>1.0/4.0</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

The “price” of modifying ‘\( T \)’ for HP superheated steam -or its effect on the objective function
value- can be obtained from,

\begin{equation}
    f + \lambda \delta T
\end{equation}

where \( f \) is the objective function value, \( \lambda \) is the Lagrange multiplier value (in this case for the HP steam temperature) and \( \delta T \) is the differential change (in HP steam temperature for this example).

For the original 'two turbine model' HP steam \( T=550 \, ^\circ C \) was a fixed variable, upon solution of the problem \( \lambda = -0.1717 \times 10^{-3} \) was obtained while the optimised thermal efficiency \(^1\) was \( f = -0.282695 \).

Applying equation (7.5) the predicted objective function value at HP steam \( T=551 \, ^\circ C \) (\( f_{551^\circ C} \)) is,

\[ f_{551^\circ C} = -0.282695 + \left[(-0.1717 \times 10^{-3})(+1.0)\right] = -0.282867 \]

Similarly, the predicted objective function value at HP steam \( T=549 \, ^\circ C \) (\( f_{549^\circ C} \)) is,

\[ f_{549^\circ C} = -0.282523 \]

In both cases the use of the 'shadow price' concepts predicted very well the calculated optimised objective function (see Table 7.7).

Since the predicted change in objective function using equation (7.5) agrees with that obtained using the SQP optimiser, then it is concluded that filterSQP is correctly calculating the multipliers for the example presented.

This simple 'shadow price' example shows that the SQP optimiser can perform efficient parametric sensitivity analysis, as would be expected in an LP or NLP code which reports multipliers. For small moves, this avoids the need to perform sensitivity analysis by repeated simulation as in modular approach to utility systems.

7.4 Energy optimisation of a single pressure steam combined cycle

In this problem, we consider a single pressure steam combined cycle. The corresponding flow-sheet is given in Fig. 7.4. The steam-cycle part of this system is given by the 'two turbine

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\(^1\) note that for the SQP optimiser the thermal efficiency was expressed as fractional negative value, since the solver minimises objective functions.
model' (Section 7.3), but the source of heat for steam generation is the exhaust gas from a LM 6000 gas turbine.

The starting guess for this system was obtained by solving the simulation problem in Chapter 6, Section 6.6.2.

In this problem, the objective is to maximise the plant thermal efficiency $\eta_h$ subject to the plant model. For this combined cycle, the plant thermal efficiency is given by,

$$ \eta_h = \frac{W_1 + W_2 + W_3}{Q_{fuel}} $$

where $W_i$ is the turbines power output ($i = 1, 2, 3$), i.e. two steam turbines and the gas turbine, and $Q_{fuel}$ is the heat added by the natural gas used in the gas turbine.

For this system we solved 5 optimisation problems. They have a different set of free variables. However, all of those problems have the following common set of 7 free variables (see also Fig. 7.4):

- OUT-stream pressure from HP and LP steam turbines;
- Mass flow to LP steam turbine (from a total of 10 kg/s fixed for HP turbine);
- Cooler heat load (or OUT-stream temperature). Bounds for cooler OUT-stream are $T \geq 50^\circ C$ and $q \geq 1.0$);
- Heat recovery (HR) exchangers heat load (economiser, evaporator and superheater).  

The 5 energy optimisation problems consider the above-mentioned free variables and different combinations of free/fixed 'T' and 'P' for the HP superheated steam (see Table 7.8).

Important bounds on variables include:

- pumps IN-stream $q \geq 1.0$
- HR exchangers approach temperatures $DT \geq 5.0^\circ C$ for problems 'i - iv', and $DT \geq 8.5^\circ C$ for 'problem v' in Table 7.8.

The plant model for this combined cycle has 446 variables and 319 constraints, according to our modelling system, FMS. From there we have up to 9 free variables and at least 118 specifications

\[2\text{ The product 'UA' in the heat transfer equation is also obtained within the optimisation.}\]
Figure 7.4: Single pressure steam combined cycle.
(depending on the optimisation example). The relevant fixed variables are selected as in this plant simulation (Chapter 6, Section 6.6.2), in addition for problems 'i - iv' in Table 7.8 we fixed the economiser outlet temperature (see also Fig. 7.4). 'Problem v' (with free HP steam ‘T’ and ‘P’) has the economiser outlet temperature as free variable, to allow the optimum pressure to be found within the feasible bounds, basically bounds on approach temperatures in HR exchangers.

Results for the 5 optimisation examples are shown in Table 7.8, where we also show the values of some optimised variables.

7.4.1 Analysis of results for energy optimisation problems

In the 5 optimisation examples solved we show the effect of HP superheating steam ‘T’ and ‘P’ on the plant thermal efficiency. As we expected the highest optimised ‘T’ and ‘P’ for HP steam produce the highest thermal efficiency (of up to 50.59% for ‘problem v’ in Table 7.8).

What is very important to note here, is the ability of both the proposed model and the NLP optimiser to predict the plant energy performance under a different set of free variables, the most complex being ‘problem v’, where having P and T for HP steam as decision variables, we found and optimal solution at the highest feasible P and T under the bounds on variables.

The highest optimal pressure and temperature in ‘problem v’ were limited by the lower bound given to the HR exchangers’ approach temperatures \( DT \geq 8.5°C \). For example the \( DT_h \) (see heat recovery exchanger model in Appendix D, Section D.3) for the superheater in Fig. 7.4 is the difference between the hot side IN-stream \( T \) (gas turbine exhaust at 473 °C) minus the cold side OUT-stream \( T \) (optimum HP superheated steam \( T=464.5°C \)), see ‘problem v’ in Table 7.8. A similar situation was found for the optimal HP steam \( P \), but in this case it was limited by the HP saturation temperature, producing a \( DT_c = 8.5°C \) (obtained by the difference between the evaporator hot side OUT-stream and the evaporator cold side IN-stream).

It is interesting to note that under this energy optimisation model, our modelling variables include optimum heat loads and ‘UA’ (product of overall heat transfer coefficient and heat transfer area) for each of the HR exchangers.

After successful solution of energy optimisation problems, we solved economic optimisation problems beginning in the next section.
<table>
<thead>
<tr>
<th>Problem</th>
<th>i</th>
<th>ii</th>
<th>iii</th>
<th>iv</th>
<th>v</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP superheated steam conditions:</td>
<td>( T = 468 , ^\circ C )</td>
<td>( T = 468 , ^\circ C )</td>
<td>( T = 468 , ^\circ C )</td>
<td>( T = 468 , ^\circ C )</td>
<td>( T = 464.5 , ^\circ C )</td>
</tr>
<tr>
<td>( P ) (fixed) ( ) [MPa]</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>4.5</td>
<td>3.042</td>
</tr>
<tr>
<td>Cooler heat load ( Q ) [kW]</td>
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<td>-23,295</td>
<td>-21,310</td>
<td>-22,189</td>
<td>-20,678</td>
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<td>181.3</td>
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<td>351.4</td>
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<td>ii</td>
<td>iii</td>
<td>iv</td>
<td>v</td>
</tr>
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<td></td>
</tr>
<tr>
<td>Q/UA, [kW]/[kW/°C]</td>
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</tr>
<tr>
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<td>5.99/107.0</td>
<td>5.992/107.5</td>
<td>5.992/107.5</td>
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</tr>
<tr>
<td>LP turbine OUT-stream ( F ), [MPa]</td>
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<tr>
<td>0.0123</td>
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<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td></td>
</tr>
<tr>
<td>Initial value ( f(x^*) ):</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>153.0</td>
<td>153.0</td>
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<td>Optimised variables:</td>
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<td>HP turbine OUT-stream ( P ) [MPa]</td>
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<td></td>
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<td>LP turbine OUT-stream ( F ), [MPa]</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>0.0123</td>
<td>0.0123</td>
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<td>0.0123</td>
<td>0.0123</td>
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<td></td>
</tr>
<tr>
<td>Final value ( f(x^*) ):</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-0.4930</td>
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<td>0.0123</td>
<td>0.0123</td>
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<td>Gradient evaluations:</td>
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<td>1</td>
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<td>Total number of QP pivots:</td>
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<td>2,931</td>
<td>3,410</td>
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<td>6,329</td>
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<td>-0.4909</td>
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<td>HP turbine OUT-stream ( F ), [MPa]</td>
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<td>Steam flow, [kg/s] to LP turbine</td>
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<td>10.0</td>
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<td>10.0</td>
<td>10.0</td>
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<tr>
<td>Cooler heat load ( Q ) [kW]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>9</td>
<td>10</td>
<td>20</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>of which iterations in inf. NLP: 5</td>
<td>1</td>
<td>5</td>
<td>7</td>
<td>4</td>
<td>4</td>
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<td>Q/UA, [kW]/[kW/°C]</td>
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<td>Economiser:</td>
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</tr>
<tr>
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<td>5.992/107.5</td>
<td>5.99/107.0</td>
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<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td></td>
</tr>
<tr>
<td>5.99/107.0</td>
<td>5.992/107.5</td>
<td>5.99/107.0</td>
<td>5.992/107.5</td>
<td>5.992/107.5</td>
<td></td>
</tr>
<tr>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td>0.0123</td>
<td></td>
</tr>
</tbody>
</table>

Table 7.8: Results of problems for energy optimisation of a single pressure steam combined cycle.
7.5 Combined cycle power plant with two steam pressure levels.

This is a complex system to optimise which considers economic optimisation problems for a combined cycle power plant with two steam pressure levels (shown in Fig. 7.5). The system has a steam injected gas turbine (SIGT), a heat recovery steam generator (HRSG) producing LP steam for deaeration purposes and HP steam for power generation in two steam turbines (the HP and the LP turbines), a deaerator, pumps, valves, a water/water heat exchanger and an air-cooled condenser.

This plant has a realistic pump model (given in Appendix D, Section D.8) and does not make the simplification used in previous optimisation models (Sections 7.3 - 7.4) where we use the 'valve' model for pumps, effectively neglecting pump power requirements.

Given the complexity of this system and the fact that this was the first economic optimisation model solved using FMS and the filterSQP code, we decided to do two optimisation problems related to this plant. Details are given in the following two sections.

7.5.1 Economic optimisation of the Rankine cycle-part

The flowsheet for this optimisation problem was presented in Chapter 6, Fig. 6.11 on page 128 and is the steam cycle-part in Fig. 7.5, i.e. does not include the gas turbine, nor the HRSG, but the rest of the equipment. For this problem there are 392 variables and 320 constraints.

In this optimisation problem we consider an economic objective function involving capital and operating cost. Our objective is to minimise the cost of equipment and external utilities (HP and LP steam in this example) while producing the maximum electric power from the steam turbines. Thus, for this problem we use our 'general economic objective function' (given in Chapter 3, Section 3.4.2):

\[
O.F. = - \left[ (Op. \text{ Incomes} - Op. \text{ Expenses}) - r \left( \text{Capital Costs} \right) \right]
\]

where 'Op. Incomes' are the annual (k US $/year) operating revenues from selling electricity (produced from the two steam turbines); 'Op. Expenses' are the variable costs from turbines operating and maintenance, from buying external utilities (makeup water, HP and LP steam) and from power consumed by pumps and by the air-cooled condenser; finally 'Capital Costs' are
Figure 7.5: Double pressure steam combined cycle.
considered for all the major equipment units: steam turbines, deaerator, pumps, water/water heat exchanger and air-cooled condenser. Note that in this problem, the water/water heat exchanger has 'U' and 'A' as separate variables, since the cost function for this unit is a function of 'A'.

**Fully constrained model**

A first numerical experiment consisted in solving the fully constrained model with filterSQP. This implied the specification of fixed values for all the plant's degrees of freedom (as in the simulation of this flowsheet, Chapter 6, Section 6.5.4). Using a warm-guess obtained by simulation with the sparse NLAE solver, the fully constrained model was solved by filterSQP in 4 iterations (see Table 7.9).

For the fully constrained model we have $392 - 320 = 82$ fixed variables which include unit and streams modelling variables as well as specifications for economic calculations, component identification in gas streams and number of IN/OUT streams in mixers and splitters.

**Passing from simulation to optimisation**

In order to solve the economic optimisation problem for this plant section of the combined cycle we select the following 7 free variables (see also Fig. 7.5):

<table>
<thead>
<tr>
<th>stream</th>
<th>freed variable</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>LP steam to deaerator:</td>
<td>$F_1$, [kg/s]</td>
<td>0.77 - 3.0</td>
</tr>
<tr>
<td>HP steam to HP turbine:</td>
<td>$F_2$, [kg/s]</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>HP turbine OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>0.07 - 12.5</td>
</tr>
<tr>
<td>LP turbine IN-stream:</td>
<td>$F_3$, [kg/s]</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>LP turbine OUT-stream:</td>
<td>$P_1$, [MPa]</td>
<td>$1.0 \times 10^{-4} - 12.5$</td>
</tr>
<tr>
<td>Valve 'V4' IN-stream:</td>
<td>$F_4$, [kg/s]</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>Heat exchanger 'HX 1' hot side OUT-stream:</td>
<td>$T$, [°C]</td>
<td>10.0 - 500.0</td>
</tr>
</tbody>
</table>

Results for the optimisation of this steam system-part of the combined cycle along with the optimised variables are presented in column 3 of Table 7.9. Recall that this model contains a water/water heat exchanger aimed to preheat water with deaerated water in order to minimise LP steam for deaeration (see Fig. 7.5). As can be noticed in those results, for this particular situation (see characteristics of heat exchanger 'HX 1' in the lower part of Table 7.9), investing in a heat exchanger to heat-up water for the deaerator in 0.2°C does not seems to be wise. Consequently, under the problem conditions, our flowsheet will not consider such a
Table 7.9: Results of problems for economic optimisation of the steam system-part of a double pressure steam combined cycle.

<table>
<thead>
<tr>
<th>Example:</th>
<th>fully constrained model</th>
<th>model with exchanger 'HX 1'</th>
<th>model without exchanger 'HX 1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>102.2</td>
<td>347.1</td>
<td>205.9</td>
</tr>
<tr>
<td>Iterations:</td>
<td>4</td>
<td>21</td>
<td>14</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>2</td>
<td>10</td>
<td>4</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>5</td>
<td>30</td>
<td>27</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>1,712</td>
<td>5,391</td>
<td>4,330</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>3</td>
<td>20</td>
<td>21</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>6</td>
<td>31</td>
<td>27</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>5</td>
<td>19</td>
<td>12</td>
</tr>
<tr>
<td>Final value f(x*), [k$/year]:</td>
<td>11,155.354</td>
<td>7,146.329</td>
<td>7,126.099</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>50/100</td>
<td>0.1/0.656</td>
<td>0.1/0.278</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Optimised variables:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LP steam to deaerator F, [kg/s]:</td>
<td></td>
<td>0.77</td>
<td>0.77</td>
</tr>
<tr>
<td>HP steam to HP turbine F, [kg/s]:</td>
<td></td>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>HP turbine OUT-stream P, [MPa]:</td>
<td></td>
<td>0.0905</td>
<td>0.331</td>
</tr>
<tr>
<td>LP turbine IN-stream F, [kg/s]:</td>
<td></td>
<td>9.157</td>
<td>9.819</td>
</tr>
<tr>
<td>LP turbine OUT-stream P, [MPa]:</td>
<td></td>
<td>0.0123</td>
<td>0.0123</td>
</tr>
<tr>
<td>Valve 'V4' IN-stream F, [kg/s]:</td>
<td></td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Heat exchanger 'HX 1' hot side IN/OUT T, [°C]</td>
<td></td>
<td>83.3/83.1</td>
<td></td>
</tr>
<tr>
<td>Heat exchanger 'HX 1' cold side IN/OUT T, [°C]</td>
<td></td>
<td>78.1/78.3</td>
<td></td>
</tr>
<tr>
<td>Heat exchanger 'HX 1' A/Q, [m²/kW]</td>
<td></td>
<td>1.403/10.0 (at l. bound)</td>
<td></td>
</tr>
<tr>
<td>'Pump B' P //W, [kW]</td>
<td></td>
<td>7.494</td>
<td>0.0</td>
</tr>
</tbody>
</table>
heat exchanger. Then, the next problem was to optimise this steam cycle-part of the combined
cycle, but without having the water/water heat exchanger ‘HX 1’. Results for this problem
(see column 4 of Table 7.9) confirm the lowest value for the objective function among the
experiments on this subsystem optimisation.

It is important to mention that in all converged solutions for this sub-system of the combined
cycle, the optimum mass flow through valve ‘V4’ in Fig. 7.5 has a value of 0.0 kg/s (at the lower
bound) and the OUT-stream of this valve converged to an spurious temperature (consequently
producing spurious $h_2$ and $s_2$). This is because the valve energy balance $H_2 = H_1$ cannot be
solved for $h_2$ at zero mass flow. However, these results having $F_2 = 0.0$ do not affect at all
further calculations in unit models/streams within the flowsheet.

7.5.2 Economic optimisation of the whole combined cycle (dense vs.
sparse filterSQP versions)

In this optimisation problem we do not consider the water/water heat exchanger (see Fig. 7.6)
which was economically unnecessary when we optimised the steam cycle-part of this plant in
Section 7.5.1. In addition, for this example we do not consider the HRSG capital cost. We use
cost functions for heat recovery exchangers only in the solution of MINLP problems (Section
7.7 and Chapter 8).

We compared the performance of the filterSQP dense vs. the sparse versions (for the ‘two
turbine model’ in Section 7.3.2), and now we do this comparison for a complex model.

Again as in Section 7.5.1 we use our ‘general economic objective function’ (Chapter 3, Sec-
tion 3.4.2), but now the capital and operating costs are calculated with respect to the flowsheet
in Fig. 7.6. The objective is to minimise the annual cost of the plant.

According to FMS, this model has 797 variables and 597 constraints. From the 797 variables
680 are stream and unit variables, the rest are for component identification for gas streams, for
the number of input/output streams for mixers and splitters and for economic parameters. For
this optimisation problem we have the following 7 free variables:
Using the warm guess from the simulation of the whole system, the economic optimisation problem converged according to the results shown in Table 7.10, where both the dense and the sparse filterSQP versions are compared.

The optimised variables from both the dense and the sparse versions are shown in Table 7.11.

From the results shown in Table 7.10 note the big difference in computing time between the dense and the sparse filterSQP versions. The dense version spent about 207 seconds/iteration while the sparse version spent about 9.2 seconds/iteration. The difference between the number of iteration is not too large (16 and 9 respectively), but the number of QP pivots (8723 and 475

<table>
<thead>
<tr>
<th>stream</th>
<th>freed variable</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>LP steam to deaerator:</td>
<td>$F$, [kg/s]</td>
<td>0.87 - 3.0</td>
</tr>
<tr>
<td>HP steam to HP turbine:</td>
<td>$F$, [kg/s]</td>
<td>6.0 - 20.0</td>
</tr>
<tr>
<td>HP steam to HP turbine:</td>
<td>$T$, [°C]</td>
<td>400.0 - 500.0</td>
</tr>
<tr>
<td>HP turbine OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>$1.0 \times 10^{-4}$ - 12.5</td>
</tr>
<tr>
<td>LP turbine IN-stream:</td>
<td>$F$, [kg/s]</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>LP turbine OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>$1.0 \times 10^{-4}$ - 12.5</td>
</tr>
<tr>
<td>Make up water:</td>
<td>$F$, [kg/s]</td>
<td>3.65 - 8.0</td>
</tr>
</tbody>
</table>

Figure 7.6: Double pressure steam combined cycle for economic optimisation.
for the dense and sparse versions respectively) makes the big difference in computing time. The difference in \( f(x^*) \) values (0.031%) produces similar values for the optimised variables shown in Table 7.11. However, the HP turbine OUT-stream pressure converged to a spurious value (0.0357 MPa) considering practical inlet pressures for the LP turbine. The use of a lower bound for HP turbine OUT-stream pressure, given by the design practice, is advisable.

Although it is clear that large-scale problems are not tractable with a dense version of a NLP optimiser, this example illustrates the efficient performance of the sparse filterSQP version for a relatively large model (with nearly 800 modelling variables).

Table 7.10: Economic optimisation of a double pressure steam combined cycle (dense and sparse filterSQP versions).

<table>
<thead>
<tr>
<th>FilterSQP</th>
<th>Dense version</th>
<th>Sparse version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>3,305.67</td>
<td>83.15</td>
</tr>
<tr>
<td>Iterations:</td>
<td>16</td>
<td>9</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>21</td>
<td>11</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>8,723</td>
<td>475</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>13</td>
<td>5</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>15</td>
<td>10</td>
</tr>
<tr>
<td>Final value ( f(x^*) ), [k$/year]:</td>
<td>4,909.8</td>
<td>4,911.319</td>
</tr>
<tr>
<td>Initial/final TR size</td>
<td>0.1/3.2</td>
<td>0.1/1.6</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 7.11: Optimised free variables for a two pressure steam combined cycle.

<table>
<thead>
<tr>
<th>filtersQP version:</th>
<th>Optimised variable</th>
<th>Dense</th>
<th>Sparse</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>LP steam to deaerator ( F_i ), [kg/s]:</td>
<td></td>
<td>2.094</td>
<td>2.212</td>
<td>0.87 - 7.0</td>
</tr>
<tr>
<td>HP steam to HP turbine ( F_i ), [kg/s]:</td>
<td></td>
<td>6.852</td>
<td>6.852</td>
<td>6.0 - 20.0</td>
</tr>
<tr>
<td>HP steam to HP turbine ( T_i ), [°C]:</td>
<td></td>
<td>400.0</td>
<td>400.0</td>
<td>400.0 - 500.0</td>
</tr>
<tr>
<td>HP turbine OUT-stream ( P_i ), [MPa]:</td>
<td></td>
<td>0.0357</td>
<td>0.331</td>
<td>( 1.0 \times 10^{-4} - 12.5 )</td>
</tr>
<tr>
<td>LP turbine IN-stream ( F_i ), [kg/s]:</td>
<td></td>
<td>6.521</td>
<td>6.658</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>LP turbine OUT-stream ( P_i ), [MPa]:</td>
<td></td>
<td>0.0123</td>
<td>0.0123</td>
<td>( 1.0 \times 10^{-4} - 12.5 )</td>
</tr>
<tr>
<td>Make up water ( F_i ), [kg/s]:</td>
<td></td>
<td>4.211</td>
<td>4.211</td>
<td>3.654 - 8.0</td>
</tr>
</tbody>
</table>
7.6 Optimisation problems for a real cogeneration plant

Here we present a set of 3 complex profit optimisation problems based on the model for a real cogeneration plant currently in operation (Gator-Power, 1994). The corresponding flowsheet is presented in Fig. 7.7. For the solution of the profit optimisation problems, we provide a warm starting point obtained by the plant simulation (Chapter 6, Section 6.6.4).

This cogeneration plant has a gas turbine (a General Electric LM 6000) with steam injection for electric power generation. The turbine exhaust is the source of heat for a HRSG where steam at three different pressure levels is produced. Low pressure (LP) steam is used for deaeration purposes and for LP steam heating demands; intermediate pressure (IP) steam is generated for satisfying heating demands for 'steam load II' in Fig. 7.7; and, high pressure (HP) steam is generated for steam injection to the gas turbine and for HP steam demand for 'steam load I' in Fig. 7.7. The HRSG contains 11 heat recovery exchangers. The plant has two water/water heat exchangers that are used for preheating the condensate to be deaerated thus minimising the LP steam needed to deaerate the condensate.

Some details on the steam levels include:

- HP steam is produced at 5.127 MPa and 382.4 °C. In the base case design 6.54 kg/s are exported (we assume a selling cost, given by cost functions in Appendix E, Section E.1) and 3.654 kg/s are used for steam injection to the gas turbine.

- IP steam is produced at 0.7908 MPa and 208.5 °C to be exported at certain selling price. In the base case design we produce 3.13 kg/s of steam at IP.

- LP steam is produced at 138.1 °C saturated. The base case considers 1.73 kg/s, part of this LP steam is used for the deaerator (1.68 kg/s) and the rest (0.05 kg/s) is exported.

In the simulation of the base case design (presented in Chapter 6, Section 6.6.4) we have reproduced the plant performance including steam conditions \( F, T, P \) as given through all the heat recovery exchangers in the HRSG at each pressure level and throughout the plant (where the information was available (Gator-Power, 1994)).

The FMS model for SQP optimisation has 1467 variables and 1147 equations. In problems presented below we have from 4 to 9 free variables, so there are from 316 to 311 specifications respectively.
Figure 7.7: Cogeneration plant for profit optimisation problems.
7.6.1 Profit optimisation problems

Since the cogeneration plant for this complex examples is currently in operation we do not consider capital costs. We propose an objective function \( O.F. \) aimed to maximise the annual net revenue obtained by selling electric power and steam minus the annual cost of purchasing the external utilities like fuel and makeup water and also operating and maintenance costs.

We present 3 optimisation examples for the operating costs and revenues for the “cogeneration plant” at The University of Florida (Gator-Power, 1994), thus showing how filterSQP, the models and FMS work on solving industrial size real problems. Again, from our ‘general economic objective function’ (Chapter 3, Section 3.4.2) we have:

\[
O.F. = \left( Income - Expenses \right)
\]

where,

\[
Income = Sales \ of \ Net \ Power \ produced + Sales \ of \ Steam \ produced
\]

and,

\[
Net \ Power \ produced = Gas \ Turbine \ output - pumping \ power
\]

\[
Expenses = \$ \ Fuel + \$ \ demineralised \ makeup \ water + \$ \ Operating \ and \ Maintenance
\]

This \( O.F. \) is optimised subject to the constraints given by the plant model and bounds on variables. For instance, stack temperature \(^3\) is limited by the acid dew point of the exhaust gases (Ganapathy, 1991) so it should be higher than that value in order to avoid stack corrosion. For the optimisation examples a value of 106 °C is considered as the lower bound on the HRSG exhaust gases. This value was taken from a study reported on HRSG performance where a complex model is used to compare operating data from full-scale units using natural gas (Ong’iro \textit{et al.}, 1997). In addition for the optimisation examples it is considered that,

- the gas turbine is operating at its nominal capacity;
- the HP steam sold is the HP steam that goes to the desuperheater \( \# 1 \) (DSH \( \# 1 \) in Fig. 7.7);
- the IP steam sold is all the IP steam generated which goes to the desuperheater \( \# 2 \) (DSH \( \# 2 \) in Fig. 7.7);

\(^3\) is the exhaust temperature at the outlet of the HRSG.
• the LP steam sold is the difference between the whole LP steam produced and the mass flow required for the deaerator;

• Condensate from the steam loads I and II in Fig. 7.7 is returned at \( T = 55 \, ^\circ\text{C} \);

• Ambient temperature and make up water supply \( T = 27 \, ^\circ\text{C} \).

The simulation of the whole cogeneration plant involved full specification of the Degrees of Freedom. In the optimisation problems below a progressive increase in free variables is considered from one example to the next.

Example i

Table 7.12 gives the free variables considered for this optimisation problem (see also Fig. 7.7). Here ‘HX 1’ and ‘HX 2’ are the water/water heat exchangers used to preheat the condensate before it goes to the deaerator and the ‘deaerated water’ refers to the Deaerator water OUT-stream that goes to pumps. The optimisation problem with these free variables will show the effect of optimising the preheating condensate conditions as well as the LP steam used for deaeration purposes. Table 7.13 shows the optimised variables after the profit optimisation problem was solved.

A few important operating variables obtained as a result of the optimised solution in this

Table 7.12: Free variables for profit optimisation of the cogeneration plant (Example i).

<table>
<thead>
<tr>
<th>stream</th>
<th>freed variable</th>
<th>simulation fixed value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water to valve V4:</td>
<td>( F, [\text{kg/s}] )</td>
<td>( 1.0 \times 10^{-8} )</td>
<td>0.0 - 20.0</td>
</tr>
<tr>
<td>HX 1 hot side OUT-stream:</td>
<td>( T, [\degree\text{C}] )</td>
<td>65.56</td>
<td>10.0 - 200.0</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream:</td>
<td>( T, [\degree\text{C}] )</td>
<td>82.78</td>
<td>50.0 - 400.0</td>
</tr>
<tr>
<td>Deaerated water:</td>
<td>( T, [\degree\text{C}] )</td>
<td>110.0</td>
<td>50.0 - 200.0</td>
</tr>
</tbody>
</table>

Table 7.13: Optimised variables for the profit optimisation of the cogeneration plant (Example i).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water to valve V4 ( F, [\text{kg/s}] ):</td>
<td>0.0</td>
<td>( 1.0 \times 10^{-8} )</td>
</tr>
<tr>
<td>HX 1 hot side OUT-stream ( T, [\degree\text{C}] ):</td>
<td>47.9</td>
<td>65.56</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream ( T, [\degree\text{C}] ):</td>
<td>52.6</td>
<td>82.78</td>
</tr>
<tr>
<td>Deaerated water ( T, [\degree\text{C}] ):</td>
<td>59.9</td>
<td>110.0</td>
</tr>
</tbody>
</table>
Example ii

This example consider the free variables of ‘Example i’ (except mass flow to valve ‘V4’) as well as the water mass flows to the HP/IP/LP steam generating systems. Table 7.15 gives the 6 variables that were freed for this optimisation ‘Example ii’ along with the corresponding former fixed values used in the simulation of the plant.

Table 7.16 shows the optimised variables at the optimised solution of ‘Example ii’. In Table 7.17 are shown a few important operating variables obtained as a result of the optimised solution

Table 7.14: Relevant operating variables for the profit optimisation of the cogeneration plant (Example i).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP steam sold $F$, [kg/s]:</td>
<td>6.486</td>
<td>6.504</td>
</tr>
<tr>
<td>IP steam sold $F$, [kg/s]:</td>
<td>3.023</td>
<td>3.13</td>
</tr>
<tr>
<td>LP steam sold $F$, [kg/s]:</td>
<td>0.545</td>
<td>0.04183</td>
</tr>
<tr>
<td>stack temperature, [°C]:</td>
<td>115.6</td>
<td>124.4</td>
</tr>
<tr>
<td>LP steam for Deaeration $F$, [kg/s]:</td>
<td>0.995</td>
<td>1.68</td>
</tr>
</tbody>
</table>

Table 7.15: Free variables for the profit optimisation of the cogeneration plant (Example ii).

<table>
<thead>
<tr>
<th>stream</th>
<th>freed variable</th>
<th>simulation fixed value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX 1 hot side OUT-stream:</td>
<td>$T$, [°C]</td>
<td>65.56</td>
<td>10.0 - 200.0</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream:</td>
<td>$T$, [°C]</td>
<td>82.78</td>
<td>50.0 - 200.0</td>
</tr>
<tr>
<td>Deaerated water:</td>
<td>$T$, [°C]</td>
<td>110.0</td>
<td>50.0 - 200.0</td>
</tr>
<tr>
<td>Water to HP economiser 3:</td>
<td>$F$, [kg/s]</td>
<td>10.312</td>
<td>5.0 - 20.0</td>
</tr>
<tr>
<td>Water to IP economiser:</td>
<td>$F$, [kg/s]</td>
<td>3.225</td>
<td>1.0 - 5.0</td>
</tr>
<tr>
<td>Water to LP steam drum:</td>
<td>$F$, [kg/s]</td>
<td>1.730</td>
<td>1.5 - 3.0</td>
</tr>
</tbody>
</table>

Table 7.16: Optimised variables for the profit optimisation of the cogeneration plant (Example ii).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX 1 hot side OUT-stream $T$, [°C]:</td>
<td>47.3</td>
<td>65.56</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream $T$, [°C]:</td>
<td>51.1</td>
<td>82.78</td>
</tr>
<tr>
<td>Deaerated water:</td>
<td>56.9</td>
<td>110.0</td>
</tr>
<tr>
<td>Water to HP economiser 3 $F$, [kg/s]:</td>
<td>10.138</td>
<td>10.312</td>
</tr>
<tr>
<td>Water to IP economiser $F$, [kg/s]:</td>
<td>3.07</td>
<td>3.225</td>
</tr>
<tr>
<td>Water to LP steam drum $F$, [kg/s]:</td>
<td>1.561</td>
<td>1.730</td>
</tr>
</tbody>
</table>
Table 7.17: Relevant operating variables for the profit optimisation of the cogeneration plant (Example ii).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP steam sold $F_1$, [kg/s]:</td>
<td>6.506</td>
<td>6.504</td>
</tr>
<tr>
<td>IP steam sold $F_2$, [kg/s]:</td>
<td>3.07</td>
<td>3.13</td>
</tr>
<tr>
<td>LP steam sold $F_3$, [kg/s]:</td>
<td>0.654</td>
<td>0.04183</td>
</tr>
<tr>
<td>stack temperature, [°C]:</td>
<td>116.0</td>
<td>124.4</td>
</tr>
<tr>
<td>LP steam for Deaeration $F_4$, [kg/s]:</td>
<td>0.907</td>
<td>1.68</td>
</tr>
</tbody>
</table>

Table 7.18: Free variables for the profit optimisation of the cogeneration plant (Example iii).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>freed variable</th>
<th>fixed value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX 1 hot side OUT-stream:</td>
<td>$T$, [°C]</td>
<td>65.56</td>
<td>10.0 - 200.0</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream:</td>
<td>$T$, [°C]</td>
<td>82.78</td>
<td>50.0 - 200.0</td>
</tr>
<tr>
<td>Deaerated water:</td>
<td>$T$, [°C]</td>
<td>110.0</td>
<td>50.0 - 200.0</td>
</tr>
<tr>
<td>HP pump OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>5.348</td>
<td>5.1 - 6.0</td>
</tr>
<tr>
<td>LP/IP pump OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>0.846</td>
<td>0.51 - 1.0</td>
</tr>
<tr>
<td>Water to LP steam drum:</td>
<td>$P$, [MPa]</td>
<td>0.343</td>
<td>0.1289 - 0.35</td>
</tr>
<tr>
<td>Water to HP economiser 3:</td>
<td>$F$, [kg/s]</td>
<td>10.312</td>
<td>5.0 - 20.0</td>
</tr>
<tr>
<td>Water to IP economiser:</td>
<td>$F$, [kg/s]</td>
<td>3.225</td>
<td>1.0 - 5.0</td>
</tr>
<tr>
<td>Water to LP steam drum:</td>
<td>$F$, [kg/s]</td>
<td>1.730</td>
<td>1.5 - 3.0</td>
</tr>
</tbody>
</table>

in this example.

**Example iii**

The last profit optimisation example considers all the free variables given for the 'Example ii' plus the HP/IP/LP steam generating pressures, giving a total of 9 free variables for optimisation. Table 7.18 gives the variables that were freed for this optimisation 'Example iii', while Table 7.19 shows the optimised variables at problem solution.

Some important operating variables obtained as a result of the optimised solution in this example are shown in Table 7.20. Note that the optimum stack temperature is in the lower bound given i.e. 106 °C.

### 7.6.2 Results and discussion of the profit optimisation problems

In Table 7.21 we show the performance of the sparse filterSQP for these three Examples (i, ii, iii). It should be noted that since the NLP optimiser minimises objective functions, we use a
'negative profit' as our economic objective function.

With regard to the solution of the optimisation Examples (i to iii), to Table 7.21 and to the tables for the optimised variables and relevant associated plant variables we can make some

Table 7.19: Optimised free variables for the profit optimisation of the cogeneration plant (Example iii).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX 1 hot side OUT-stream $T$, [$^\circ$C]:</td>
<td>53.9</td>
<td>65.56</td>
</tr>
<tr>
<td>HX 2 hot side OUT-stream $T$, [$^\circ$C]:</td>
<td>62.5</td>
<td>82.78</td>
</tr>
<tr>
<td>Deaerated water $T$, [$^\circ$C]:</td>
<td>76.4</td>
<td>110.0</td>
</tr>
<tr>
<td>HP pump OUT-stream $P$, [MPa]:</td>
<td>5.1</td>
<td>5.348</td>
</tr>
<tr>
<td>LP/IP pump OUT-stream $P$, [MPa]:</td>
<td>0.5702</td>
<td>0.846</td>
</tr>
<tr>
<td>Water to LP steam drum $P$, [MPa]:</td>
<td>0.171</td>
<td>0.343</td>
</tr>
<tr>
<td>Water to HP economiser 3 $F$, [kg/s]:</td>
<td>10.314</td>
<td>10.312</td>
</tr>
<tr>
<td>Water to IP economiser $F$, [kg/s]:</td>
<td>3.41</td>
<td>3.225</td>
</tr>
<tr>
<td>Water to LP steam drum $F$, [kg/s]:</td>
<td>1.928</td>
<td>1.730</td>
</tr>
</tbody>
</table>

Table 7.20: Relevant operating variables for the profit optimisation of the cogeneration plant (Example iii).

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP steam sold $F$, [kg/s]:</td>
<td>6.562</td>
<td>6.504</td>
</tr>
<tr>
<td>IP steam sold $F$, [kg/s]:</td>
<td>3.41</td>
<td>3.13</td>
</tr>
<tr>
<td>LP steam sold $F$, [kg/s]:</td>
<td>1.058</td>
<td>0.04183</td>
</tr>
<tr>
<td>stack temperature, [$^\circ$C]:</td>
<td>106.0</td>
<td>124.4</td>
</tr>
<tr>
<td>LP steam for Deaeration $F$, [kg/s]:</td>
<td>0.870</td>
<td>1.68</td>
</tr>
<tr>
<td>Deaerator operating Pressure $P$, [MPa]:</td>
<td>0.129</td>
<td>0.274</td>
</tr>
</tbody>
</table>

Table 7.21: Results from filterSQP for the profit optimisation problems (Examples i to iii).

<table>
<thead>
<tr>
<th>Filter SQP</th>
<th>Example i</th>
<th>Example ii</th>
<th>Example iii</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s)</td>
<td>3,113.2</td>
<td>1,597.1</td>
<td>620.9</td>
</tr>
<tr>
<td>Iterations:</td>
<td>47</td>
<td>21</td>
<td>6</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>90</td>
<td>43</td>
<td>8</td>
</tr>
<tr>
<td>Total number of QP pivots</td>
<td>871</td>
<td>874</td>
<td>886</td>
</tr>
<tr>
<td>Function evaluations</td>
<td>73</td>
<td>43</td>
<td>8</td>
</tr>
<tr>
<td>Constraint evaluations</td>
<td>74</td>
<td>44</td>
<td>9</td>
</tr>
<tr>
<td>Gradient evaluations</td>
<td>21</td>
<td>17</td>
<td>8</td>
</tr>
<tr>
<td>Final value $f(x^*)$, [k$/year]</td>
<td>-7,859.98</td>
<td>-7,979.19</td>
<td>-8,413.80</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>1.0/4.18 $\times 10^{-5}$</td>
<td>1.0/0.050</td>
<td>1.0/4.0</td>
</tr>
<tr>
<td>Dimension of null space</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
observations.

- FilterSQP solver performed the optimisation problems very well using a 'warm starting guess' obtained by simulation.
- The LP steam used for deaeration was minimised while the LP steam produced for selling was maximised in all the examples.
- For 'Example iii', the optimiser maximised all the HP, IP and LP steam flows produced for selling (as expected).
- 'Example iii' gave the maximum profit of all our optimisation examples on the Cogeneration Plant. The optimised pressures, flows and temperatures shows the successful implementation of our models and of filterSQP for solving this model. It is to be expected that this example, which has the most degrees of freedom, would give the most profit.
- Using a Sparc 2 workstation filterSQP spends about 66, 76, 103 seconds per iteration for problems i to iii respectively, implying for this particular model that as the number of free variables increases the time per iteration also grows.
- From experience with this three optimisation examples, we observe that as the number of free variables increased, the number of iterations decreased. This is perhaps due to the higher flexibility to move variables within the optimisation.

7.7 Using filterSQP for solving a MINLP synthesis model of HR exchangers in a combined cycle power plant

In this section we present the solution of a proposed MINLP model for the synthesis of HR exchangers in a double pressure steam combined cycle. The model is detailed in Chapter 3, Section 3.5, and the correspondent flowsheet is presented in Fig. 7.8.

Our mixed integer code named MINLP_BB (described in Chapter 4, Section 4.3) has a branch and bound strategy for the integer part of the problem and uses the filterSQP method for the continuous optimisation part. Thus, the MINLP_BB solver involves the solution of NLP optimisation problems in the first step \(^4\) and in every branch within the iterations procedure.

\(^4\) the NLP relaxation, where all modelling variables are considered continuous, as explained in Chapter 4, Section 4.3.2.
Therefore, before passing this large-scale problem directly to the MINLP_BB solver (results in Chapter 8, Section 8.3) we did some experiments on the solution of this model using only the filterSQP code.

As mentioned in Chapter 3, Section 3.5.1 the objective function for MINLP problems is given by,

\[
O.F. = - \left[ \left( Op.\ Incomes - Op.\ Expenses \right) - r \left( Capital\ Costs \right) \right] \\
- r \cdot \sum_{j=1}^{N_{HR}} C_{HR,j}
\]

(7.8)

where \( N_{HR} \) is the total number of HR exchangers in the HRSG, \( C_{HR,j} \) is the installed cost of HR exchangers and \( 'r' \) is the repayment multiplier. So the objective function consists of optimising the total annualised operating and investment costs while maximising electric power sales at 1997 prices. Thus, in equation 7.8 we have (see also Fig. 7.8):

1. **Operating Incomes** from selling electricity produced by the gas and steam turbines.
2. **Operating Expenses** incurred by fuel usage, make up water, power for air-cooled condenser fan, power for pumps, and operating and maintenance.
3. **Capital Costs** for gas turbine, steam turbines, HR exchangers, pumps, deaerator, and air-cooler condenser.

As explained in Chapter 3, Section 3.5.4 the MINLP problem consists of minimising the objective function (equation 7.8) subject by the constraints given by the plant model consisting of:

- a LM 6000 gas turbine;
- the hyperstructure for the synthesis of heat recovery (HR) exchangers in the HRSG;
- the relevant equipments for a double pressure steam system, see Fig 7.8;
- bounds on variables.

The FMS model for the optimum synthesis of this example has 3042 variables and 2139 equations. The definition of this model in FMS was not a trivial task, more details of which are given in Chapter 8, Section 8.3.
Figure 7.8: Flowsheet for the synthesis of heat recovery exchangers in a combined cycle.

*Details of hot side superstructure are given in Chapter 3, Section 3.5.3 and in Fig. 3.5
7.7.1 SQP economic optimisation of a fixed structure

The fixed structure in this model considers all the HR exchangers being in series as explained in the simulation of this model (Chapter 6, Section 6.6.5).

Fully constrained (c/s) model

We provide a warm-guess for this model obtained by simulation and solved the fully constrained model with the filterSQP code. The solution of this model was important in order to assure the valid definition of this model for solution with the filterSQP code (and consequently with the MINLP_BB solver later on). The results from filterSQP are in Table 7.22 where we show that this problem was solved in 4 iterations.

Table 7.22: MINLP synthesis model solved with filterSQP.

<table>
<thead>
<tr>
<th>Filter SQP</th>
<th>Fully c/s model</th>
<th>fixed structure</th>
<th>&quot;NLP synthesis&quot;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>806.87</td>
<td>1,004.2</td>
<td>1,370.959</td>
</tr>
<tr>
<td>Iterations:</td>
<td>4</td>
<td>26</td>
<td>38</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>QP problems solved:</td>
<td>6</td>
<td>64</td>
<td>71</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
<td>1,168</td>
<td>98</td>
<td>394</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>4</td>
<td>64</td>
<td>71</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>5</td>
<td>65</td>
<td>72</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>5</td>
<td>22</td>
<td>16</td>
</tr>
<tr>
<td>Final value f(x*), [k$/year]:</td>
<td>5,067.698</td>
<td>4,665.64</td>
<td>4,575.00587</td>
</tr>
<tr>
<td>Initial/final TR size:</td>
<td>1.0/2.0</td>
<td>8.0/1.4979</td>
<td>20.0/4.1E-6</td>
</tr>
<tr>
<td>Dimension of null space:</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Solution of the synthesis model for a fixed structure using filterSQP

From the fully constrained model we free the variables shown in Table 7.23. This example has 17 free variables.

In the process of solving this complex optimisation problem we propose the following strategy regarding the water/steam streams:

- use non-zero lower bounds (i.e. $1.0 \times 10^{-8}$) for $F$, [kg/s] to avoid singularities while the optimisation proceeds (e.g. for enthalpy flow equations within the hyperstructure). We
call this our 'zero lower bound' for mass flow in water/steam streams. Its use would not affect synthesis solutions since streams with that optimum flow do not sensibly contribute to temperature changes in mixers within an optimal structure.

The use of an initial TR ≤ 8 produced infeasible iterations which eventually made the filterSQP method to fail in the attempt to solve the problem. For a successful run an initial TR=8.0 was satisfactory. The NLP solver converged this model as shown in Table 7.22, page 181.

Table 7.24 shows the optimised variables after the cost optimisation problem was solved. In this table 'SCS' and 'MCS' denote splitters and mixers within the 'cold side superstructure' in Fig. 7.9, page 184. In this optimal solution 12.001 kg/s of HP water go to splitter 'SCS 1' (Fig. 7.9) and then distributed within the superstructure.

A few important operating variables obtained as a result of the optimised solution in this example are shown in Table 7.25.

### 7.7.2 Synthesis model solved as continuous optimisation problem

In solving this problem, we use a starting point obtained as the optimum solution from the problem solved in Section 7.7.1 for the NLP optimisation of the MINLP model for a fixed structure with 17 free variables.

For this synthesis problem, we have the 17 free variables for the solution of the MINLP model

<table>
<thead>
<tr>
<th>stream</th>
<th>freed variable</th>
<th>simulation fixed value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deaerated water:</td>
<td>$T$, [°C]</td>
<td>110.0</td>
<td>50.0 - 200.0</td>
</tr>
<tr>
<td>Deaerator operating:</td>
<td>$P$, [MPa]</td>
<td>0.3</td>
<td>0.015 - 3.0</td>
</tr>
<tr>
<td>LP steam generated:</td>
<td>$P$, [MPa]</td>
<td>0.3426</td>
<td>0.015 - 3.0</td>
</tr>
<tr>
<td>HP water for steam generation:</td>
<td>$F$, [kg/s]</td>
<td>6.61</td>
<td>9.0 - 31.0</td>
</tr>
<tr>
<td>HP Turbine OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>0.2489</td>
<td>0.07 - 12.5</td>
</tr>
<tr>
<td>LP Turbine OUT-stream:</td>
<td>$P$, [MPa]</td>
<td>0.01239</td>
<td>1.0 x 10^{-4} - 12.5</td>
</tr>
<tr>
<td>LP Turbine IN-stream:</td>
<td>$F$, [kg/s]</td>
<td>6.3</td>
<td>1.0 x 10^{-8} - 31.0</td>
</tr>
<tr>
<td>within the cold side superstructure:</td>
<td>$F$, [kg/s]</td>
<td>6.6</td>
<td>9.0 - 31.0</td>
</tr>
<tr>
<td>(this accounts for 10 mass flows detailed in Table 7.24)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 7.24: Optimised variables for the MINLP model for a fixed structure in a combined cycle (see also Fig. 7.8 - 7.9).

<table>
<thead>
<tr>
<th>Stream and Variable</th>
<th>Optimised Variable</th>
<th>Simulation Fixed Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deaerated water $T$, [$^\circ$C]:</td>
<td>57.7</td>
<td>110.0</td>
</tr>
<tr>
<td>Deaerator operating $P$, [MPa]:</td>
<td>0.018</td>
<td>0.3</td>
</tr>
<tr>
<td>LP steam generated $P$, [MPa]:</td>
<td>0.019</td>
<td>0.3426</td>
</tr>
<tr>
<td>HP water for steam generation $F$, [kg/s]:</td>
<td>12.001</td>
<td>6.61</td>
</tr>
<tr>
<td>HP Turbine OUT-stream $P$, [MPa]:</td>
<td>0.331</td>
<td>0.2489</td>
</tr>
<tr>
<td>LP Turbine OUT-stream $P$, [MPa]:</td>
<td>0.01235</td>
<td>0.01239</td>
</tr>
<tr>
<td>LP Turbine IN-stream $F$, [kg/s]:</td>
<td>11.932</td>
<td>6.3</td>
</tr>
</tbody>
</table>

within the cold side superstructure $F$, [kg/s]:
(total HP water to SCS 1 IN-stream 12.001)
SCS 1 OUT-stream.1 to MCS 1: 9.0 6.6
MCS 1 OUT-stream to HP economiser 3: 9.0 6.6
SCS 2 OUT-stream.1 to MCS 2: 9.0 6.6
MCS 2 OUT-stream to HP economiser 2: 9.0 6.6
SCS 3 OUT-stream.2 to MCS 3: 9.0 6.6
SCS 5 OUT-stream.1 to MCS 5: 11.991 6.6
MCS 5 OUT-stream to HP superheater 3: 11.991 6.6
SCS 6 OUT-stream.1 to MCS 6: 11.991 6.6
MCS 6 OUT-stream to HP superheater 2: 11.991 6.6
SCS 7 OUT-stream.2 to MCS 7: 9.0 6.6

Table 7.25: Relevant operating variables for the MINLP model for a fixed structure in a combined cycle.

<table>
<thead>
<tr>
<th>Concept</th>
<th>Optimised Value</th>
<th>Simulation Design Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>O.F.: Total cost, [k$/year]</td>
<td>4,665.644</td>
<td>5,067.598</td>
</tr>
<tr>
<td>Plant Thermal efficiency, %:</td>
<td>51.78</td>
<td>46.8</td>
</tr>
<tr>
<td>Power from HP steam turbine $W$, [kW]:</td>
<td>5,882</td>
<td>3,488</td>
</tr>
<tr>
<td>Power from LP steam turbine $W$, [kW]:</td>
<td>4,721</td>
<td>2,240</td>
</tr>
<tr>
<td>Stack temperature, °C</td>
<td>314.2</td>
<td>182.1</td>
</tr>
<tr>
<td>LP steam for Deaeration $F$, [kg/s]:</td>
<td>0.2</td>
<td>0.8149</td>
</tr>
</tbody>
</table>

for a fixed structure (Section 7.7.1) and in addition we have the following 81 free variables:

- 6 "zero flows" to allow water/steam flows through the 3 HP economisers and the 3 HP superheaters to be decided within the optimisation.
- the integer variables of all economisers and superheaters (6 variables). \(^5\)
- $T$ at outlet of HP economisers 2, 3 and of HP superheaters 1 - 3 as well as HP drum $\Delta T$ (5+1 variables).

\(^5\) For LP evaporator and HP evaporator in Fig. 7.9 we kept fixed $z = 1$. 
Figure 7.9: Cold side superstructure for the synthesis of HR exchangers in a combined cycle.

- 63 independent exhaust gas molar flows around the hot side superstructure: 7 OUT-stream flows from each of the 9 gas turbine exhaust splitters. This is because for this model, the exhaust gas splitters have 1 IN and 8 OUT-streams.

The problem has now a total of 98 free variables. The solution of this model was not as straightforward as the previous optimisation problems presented in this chapter. In this case for a successful run an initial TR=20.0 was satisfactory. The NLP solver converged this model...
Table 7.26: Optimised variables for the NLP synthesis of HR exchangers in a combined cycle.

<table>
<thead>
<tr>
<th>stream and variable</th>
<th>optimised variable</th>
<th>simulation fixed value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deaerated water, $T , ^\circ C$:</td>
<td>56.1</td>
<td>110.0</td>
</tr>
<tr>
<td>Deaerator operating $P$, [MPa]:</td>
<td>0.0166</td>
<td>0.3</td>
</tr>
<tr>
<td>LP steam generated $P$, [MPa]:</td>
<td>0.0183</td>
<td>0.3426</td>
</tr>
<tr>
<td>HP water for steam generation $F$, [kg/s]:</td>
<td>14.769</td>
<td>6.61</td>
</tr>
<tr>
<td>HP Turbine OUT-stream $P$, [MPa]:</td>
<td>0.331</td>
<td>0.2489</td>
</tr>
<tr>
<td>LP Turbine OUT-stream $P$, [MPa]:</td>
<td>0.01235</td>
<td>0.01239</td>
</tr>
<tr>
<td>LP Turbine IN-stream $F$, [kg/s]:</td>
<td>14.678</td>
<td>6.3</td>
</tr>
<tr>
<td>to HR cold side superstructure $F$, [kg/s]:</td>
<td>14.769</td>
<td>6.6</td>
</tr>
<tr>
<td>within the cold side superstructure $F$, [kg/s]:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SCS 1 OUT-stream.1 to MCS 1:</td>
<td>14.76</td>
<td>6.6</td>
</tr>
<tr>
<td>SCS 1 OUT-stream.2 to MCS 2:</td>
<td>0.009</td>
<td>–</td>
</tr>
<tr>
<td>SCS 1 OUT-stream.3 to MCS 3:</td>
<td>1.0E-8</td>
<td>–</td>
</tr>
</tbody>
</table>

as shown in Table 7.22, page 181. It should be mentioned that the solver was unable to converge the problem with initial TR values $\leq 20$, possibly for reasons discussed in Section 7.7.3.

Optimum solution description

- For this problem with 98 free variables we obtained the lowest annual cost among the three problems solved (see Table 7.22 on page 181).
- The optimal solution implies the existence of only 4 out of the 8 potential HR exchangers. The synthesised structure contains 1 HP superheater, 1 HP evaporator, 1 HP economiser and 1 LP evaporator. This is the same synthesised structure obtained with the MINLP model (in Chapter 8, Section 8.3), the corresponding flowsheet is shown there in Fig. 8.6 on page 204.
- In this solution from the filterSQP code we got $Q = 0$ for 2 of the HP superheaters as well as for 2 HP economisers in the original hyperstructure (see Fig. 7.8 on page 180). However within the solution we have $z = 1$ for these HR exchangers.
- HP steam superheated is at 300.0 $^\circ C$ (at the lower bound of HP superheated steam temperature).

Table 7.26 shows a few optimised variables after the cost optimisation problem was solved.

A few important operating variables obtained as a result of the optimised solution in this example are shown in Table 7.27.
Table 7.27: Relevant operating variables for the cost optimisation of the combined cycle synthesis problem.

<table>
<thead>
<tr>
<th>concept</th>
<th>optimised value</th>
<th>starting point</th>
</tr>
</thead>
<tbody>
<tr>
<td>O.F.: Total cost, [k$/year]</td>
<td>4,575.006</td>
<td>4,665.644</td>
</tr>
<tr>
<td>Plant Thermal efficiency, [%]:</td>
<td>52.11</td>
<td>51.78</td>
</tr>
<tr>
<td>Steam to HP steam turbine $T$, [$^\circ$C]:</td>
<td>300.0</td>
<td>450.0</td>
</tr>
<tr>
<td>Power from HP steam turbine $W$, [kW]:</td>
<td>5,853</td>
<td>5,882</td>
</tr>
<tr>
<td>Power from LP steam turbine $W$, [kW]:</td>
<td>5,070</td>
<td>4,721</td>
</tr>
<tr>
<td>stack temperature, [$^\circ$C]:</td>
<td>160.3</td>
<td>314.2</td>
</tr>
<tr>
<td>LP steam for Deaeration $F$, [kg/s]:</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

7.7.3 Discussion of results for the MINLP synthesis model solved with the NLP code

We solved three examples on the solution of the MINLP model as continuous optimisation problem using the filterSQP code. For successful solution we select a small non-zero lower bound ($1.0 \times 10^{-8}$ kg/s) for water/steam flow.

In solving this large-scale model for 0, 17 and 98 free variables, we demonstrate the ability of the modelling language FMS, and the filterSQP to tackle this complex set of problems.

The solution of the MINLP synthesis model using the filterSQP code was not as robust as the solution of previous NLP models shown in this chapter, especially for problems with 17 and 98 free variables. For these two problems initial TR values of 8.0 and 20.0 respectively were used for successful convergence, but smaller values, did not allow filterSQP to converge the model. Possible reasons may be linked with our observations in solving our synthesis models with the MINLP_BB solver in Chapter 8. Details of these are in the discussion of Section 8.4 in Chapter 8.

In spite of those difficulties, we solved successfully all our optimisation problems. In the most complex ‘NLP synthesis problem’ with 98 free variables, we found, at the solution that we need only 1 out of 3 economisers and 1 out of the 3 potential superheaters. For this problem we obtained the lowest annualised costs and the highest plant thermal efficiency of this set of three optimisation problems using the MINLP model. We also show the capability of the model and the filterSQP optimiser to work with a relatively large number of free variables.

Note that at the optimum solution for the most complex problem (with 98 decision variables) we
found heat load, cost and heat transfer area for some HR exchangers to be zero. This means that they are not present in the optimal structure, but their integer variables were not forced to be zero. This is because the use of our smoothed cost functions allowed us to successfully minimise the total cost of the systems, but the model did not enforce integer variables to be zero for HR exchangers with zero heat load. Nevertheless, we believe that this is an acceptable engineering solution to the optimisation problem, especially because it provides the optimal structure under the model considerations. Further discussion on this issue is given in Chapter 8, Section 8.4.

Finally, note that the optimised HP steam temperature for the problem with 98 free variables is 300 °C (at this variable's lower bound). This resulted from the complex combination of capital and operating costs involved in the equipment models, perhaps in an effort to minimise HR exchangers' heat transfer area within the optimal structure, while maximising HP steam mass flow whose optimal value is 14.768 kg/s (see Table 7.26).

7.8 FilterSQP performance

From the examples on the use of filterSQP presented in this chapter it can be noted that:

- Scaling variables, equations and derivative information was shown to be crucial for the efficient application of filterSQP in our utility optimisation examples. That is because the trust region does not distinguish between variables of different magnitudes.

- For the 'two turbine model' (Section 7.3) the use of a wide range of initial trust region sizes showed the success of the solver independently of the TR value. The best values of trust region was found to be 1.0 or higher since they required the least computation time and number of iterations among the trust region values tested.

- For other problems apart from the 'two turbine model' 0.1, 1.0 or higher initial trust region values worked fine.

- The filterSQP package efficiently solved optimisation problems with the accurate thermodynamic stream models.

- On the set of numerical experiments made with filterSQP it was observed that bounds on variables must be given values which prevent numerical overflows, and they should enforce physically meaningful conditions in the solution (e.g. pressure change through a steam turbines should have a lower bound of 0.0).
It was observed that the sparse filterSQP version solved problems in less iterations and in much less computation time compared to the dense filterSQP version (examples in Sections 7.3.2 and 7.5.2). Thus we show the convenience of using the sparse version for large utility problems.

In several numerical experiments on utility systems optimisation it has been found that for efficient performance of the NL optimiser filterSQP it was necessary to supply a 'warm starting guess' obtained through the solution of the simulation of the system which in our experience was done very fast and efficiently by using the sparse NLAE solver (details in Chapter 6).

Through the solution of the many NLP optimisation problems for utility systems presented in this chapter we demonstrate the capability of the proposed EO models, of the modelling system FMS and of the filterSQP package to solve difficult NLP problems. The most relevant optimisation problems are perhaps the profit optimisation of the real cogeneration plant (Section 7.6.1) for its complexity, robust solution and demonstrative application and the MINLP model solved as continuous optimisation problem, since this has more than 3,000 variables and 98 decision variables.

The computational experiments shown in this chapter allowed further assessment of the equation based utility model and the use of the new filterSQP optimiser. The overall results are very promising for the use of the sparse filterSQP version that is a robust and efficient solver for large-scale industrial size utility optimisation problems.

7.9 Summary of NLP optimisation problems

A summary on the NLP optimisation problems presented in this chapter is given in Table 7.28. There we show the total number of variables, the number of free variables, the number of constraints, the number of parameters specified and the number of iterations from the SQP solver.
Table 7.28: Summary of NLP optimisation problems.

<table>
<thead>
<tr>
<th>Problem description</th>
<th>total/free variables</th>
<th>constraints /specifications</th>
<th>iterations</th>
<th>Section in this chapter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Using the 'tolerance-tube' SQP method: (described in Chapter 4, Section 4.2.1)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Heat and Power System with steam turbines and air compressors</td>
<td>500/10</td>
<td>456/34</td>
<td>54</td>
<td>7.1</td>
</tr>
<tr>
<td>Using the filterSQP method (described in Chapter 4, Section 4.2.2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Two turbine model optimisation:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Effect of scaling example</td>
<td>130/4</td>
<td>118/9</td>
<td>unscaled:104</td>
<td>7.3.1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>scaled: 10</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10 vs. 9</td>
<td>7.3.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>from 5 to 12</td>
<td>7.3.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
<td>7.3.4</td>
</tr>
<tr>
<td>Single pressure steam combined cycle</td>
<td>446/(7 to 9)</td>
<td>319/(120 to 118)</td>
<td>from 9 to 22</td>
<td>7.4</td>
</tr>
<tr>
<td>Double pressure steam combined cycle:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- Rankine cycle-part economic optimisation</td>
<td>392/7</td>
<td>320/65</td>
<td>from 4 to 21</td>
<td>7.5.1</td>
</tr>
<tr>
<td>- Whole combined cycle economic optimisation</td>
<td>797/7</td>
<td>597/193</td>
<td>16 vs. 9</td>
<td>7.5.2</td>
</tr>
<tr>
<td>(dense vs. sparse filterSQP solvers)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A real cogeneration plant</td>
<td>1,467/(4 to 9)</td>
<td>1,147/316 to 311</td>
<td>from 6 to 47</td>
<td>7.6.1</td>
</tr>
<tr>
<td>- Profit optimisation problems</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MINLP model of HR exchangers in a combined cycle</td>
<td>3,042/(0 to 98)</td>
<td>2,139/(903 to 805)</td>
<td>4</td>
<td>7.7.1</td>
</tr>
<tr>
<td>- Fully constrained model using filterSQP</td>
<td>/0</td>
<td>/903</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- SQP economic optimisation of a fixed structure</td>
<td>/17</td>
<td>/886</td>
<td>26</td>
<td>7.7.1</td>
</tr>
<tr>
<td>- Continuous SQP synthesis</td>
<td>/98</td>
<td>/805</td>
<td>38</td>
<td>7.7.2</td>
</tr>
</tbody>
</table>
In this chapter we present the synthesis problems. Among the problems solved for this research, synthesis is the most difficult kind of problem since now we have to find the optimal flowsheet. We have identified an interesting and difficult synthesis problem consisting in finding the optimal number and position of heat recovery (HR) exchangers within a combined cycle or cogeneration plant. The MINLP synthesis model proposed for a double pressure steam generation system was presented in Chapter 3, Section 3.5. It considers the representation of alternatives in a hyperstructure involving rigorous mixing temperature calculation and all the potential HR arrangements in a heat recovery steam generator (HRSG).

We solved two synthesis models: one for a cogeneration system and one for a combined cycle power plant. Difficulties faced in solving the synthesis models as well as the solution strategy are described in Section 8.1.

For each model we provide a brief description, the number of modelling variables and equations, the insights through which we solved the problems, the results provided by the MINLP.BB solver (described in Chapter 4, Section 4.3) and a description of the synthesised solution. This chapter concludes presenting an analysis of the results.

In the solution of these synthesis problems, we use a MINLP.BB solver tolerance of $1.0 \times 10^{-4}$. 
8.1 Difficulties and solution strategy

8.1.1 Difficulties

As explained in Chapter 3, Section 3.1.1, our EO approach to utility systems involves a rigorous water/steam stream model, which has a non-smooth function (for the \( q \text{ vs. } \phi \) relationship). This function is smoothed to be continuous and differentiable. To do this we use a smoothing parameter, \( \epsilon \).

The many initial attempts made to solve our synthesis problems failed. The MINLP_BB solver reported the trust region (TR) value going below the solver tolerance as the optimisation proceeded, so no further progress could be made. One reason may be the implicit complexity of the rigorous thermopack \(^1\), another is the use of non-smooth functions in the water/steam streams (more details are given in Section 8.4 on page 207).

In some of the failed experiments the MINLP_BB solver reported a termination code “ifail=1” (finished at minimum of constraint violation), which means that the algorithm converged to a Kuhn-Tucker point of the feasibility problem (Leyffer, 1998). This indicates which constraints are causing the NLP to be (locally) infeasible as can happen if the problem has no point that satisfies the constraints. Alternatively, it may mean that the algorithm is unable to find a feasible point due to the non-convex nature of the problem. Since we first simulate a fixed structure for this model (to get a starting guess) we assessed that the model has at least one point which satisfies the constraints and hope that the MINLP_BB code may find the optimal structure.

In fact we found that, in an experiment when the MINLP_BB solver got a termination code “ifail=1” (local infeasibility), the constraints with highest residual were \( q \) vs \( \phi \) equations (the non-smooth function in the water/steam model). And very importantly, those infeasibilities were at inlet/outlet streams of HR exchangers with \( Q = 0.0 \).

8.1.2 Solution strategy

Based on our experiences, the solution of the synthesis models with the MINP_BB solver required the use of the following strategy:

\(^1\) given by highly non-linear rigorous relationships producing non-convexities.
Use of an ideal water/steam streams thermopack. This is given by (Morton, 1994b):

\[ P_{sat} = \exp \left( 17.9 - \frac{4961.0}{T + 273.15} \right) \]  

(8.1)

\[ h_L(T, P) = C_{PL} (T - T_0) + v_L (P - P_0) \]  

(8.2)

\[ h_V(T, P) = h_L(T_{nb}, P_0) + h_{vap} + C_{PV} (T - T_{nb}) \]  

(8.3)

\[ s_L(T, P) = C_{PL} \ln \left( \frac{T + 273.15}{T_0 + 273.15} \right) \]  

(8.4)

\[ s_V(T, P) = s_L(T_{nb}, P_0) + \frac{h_{vap}}{T_{nb} + 273.15} + C_{PV} \ln \left( \frac{T + 273.15}{T_{nb} + 273.15} \right) \]  

\[-R_s \ln \left( \frac{P}{P_0} \right) \]  

(8.5)

where, \( C_{PL} = 4.2 \), \( C_{PV} = 2.0 \text{ kJ/kg K}; T [\text{°C}]; h_{vap} = 2260 \text{ kJ/kg}; T_{nb} = 100.0 \text{ °C}; \) \( R_s = 0.462 \text{ kJ/kg K}; T_0 = 0.0 \text{ °C}; P_0 = 0.101325 \text{ MPa}. \) Also for the stream specific volume, we need liquid and vapour properties, taken respectively as \( v_L = 0.001 \text{ m}^3/\text{kg} \) and \( v_V \) as calculated from ideal gas equation of state.

Select a smoothing parameter (\( \epsilon \)) for the smoothed equation in the water/steam stream model to start the solution with the MINLP_BB solver. If necessary, decrease this parameter interactively until we observed satisfactory solution from the MINLP_BB solver.

To start the solution we got a warm-guess for the models through the simulation of the fully constrained synthesis model for a fixed structure. This was made by using the sparse NLAE solver and water/steam stream with ideal thermopack. We also imposed bounds as follows:

- H (enthalpy flow) lower bound was set to \( 1.0 \times 10^{-8} \text{ kW} \);

- molar flow for streams in the hot side superstructure have a lower bound of \( 1.0 \times 10^{-7} \text{ kmol/s} \);

- mass flow for the streams in the cold side superstructure have a lower bound of \( 1.0 \times 10^{-8} \text{ kg/s} \);

The use of this solution strategy provided the optimal structure from the synthesis problems presented below.
8.2 Synthesis of HP steam superheaters in a cogeneration system

This problem consists in synthesising the HR exchangers in the HRSG which is part of a cogeneration system. The cogeneration system supplies electric power from a gas turbine and HP steam superheated produced by heat recovery from the gas turbine exhaust. For this model we assume that subcooled water at temperature near the saturation point (where the actual value depends on the optimised free variables) is supplied to the HP steam generation system of this plant. This implies that we do not consider the economisers of the HRSG in the synthesis model.

A flowsheet for the cogeneration plant model, including the cold side (for water/steam streams) superstructure is shown in Fig. 8.1. This system includes:

- a gas turbine General Electric model LM 6000 operating at nominal conditions;
- a heat recovery steam generator having: 1 HP evaporator and up to 3 potential HP steam superheaters;
- HP steam drum;
- hyperstructure for considering all the synthesis alternatives with 4 HR exchangers, including:
  - Gas turbine exhaust splitters in the 'hot side' superstructure with 1 IN-stream and 4 OUT-streams (to HR exchangers);
  - Gas turbine exhaust mixers in the 'hot side' superstructure with 4 IN-streams (from potential HR exchangers) and 1 OUT-stream;
  - 'Cold side' superstructure as shown in Fig. 8.1.

The model defined in FMS has 1167 variables and 795 constraints. Considering the 31 free variables for this problem (detailed below) we have 341 specifications.

The objective function, is given by our 'general economic objective function' as explained in

---

2 details and a representation of the 'hot side' superstructure are given in Chapter 3, Section 3.5.3 on page 53.
Figure 8.1: Flowsheet for the synthesis model of HP steam superheaters in a cogeneration plant.
Chapter 3, Section 3.5.1:

\[
O.F. = - \left[ (Op. \text{ Incomes} - Op. \text{ Expenses}) - r (Capital Costs) \right. \\
\left. - r \sum_{j=1}^{N_{HR}} C_{HR,j} \right]
\]  

(8.6)

where 'Op. Incomes' are obtained from selling electricity and HP steam produced. 'Op. Expenses' are given by the purchased natural gas for the turbine and by operating and maintenance costs. 'Capital Costs' involve costs for gas turbine. The last term in equation (8.6) accounts for the capital costs of HR exchangers. 'r' is the repayment multiplier as explained in Appendix E.

Thus, the synthesis problem is to find the optimal structure of HR exchangers in the HRSG while maximising the profit defined in equation (8.6) subject to the constraints given by the MINLP plant model and by bounds on variables. We also consider important design variables as free variables, e.g. HP steam mass flow. More details are given below.

For solving this problem we obtained a warm starting guess for a fixed structure by the simulation of this model considering all \( z = 1 \) for HR exchangers operating in series. This means that 'all' gas turbine exhaust \(^3\) goes to superheater 'HP shtr 1', then to 'HP shtr 2' and to 'HP shtr 3', finally to HP evaporator (see Fig. 8.1). On the cold side superstructure, 'all' HP steam goes to 'HP shtr 3' then to 'HP shtr 2' and is exported from 'HP shtr 1' (in Fig. 8.1).

Now for the synthesis problem we want to find the optimal structure having the following 31 free variables:

- Subcooled water mass flow at HP for steam generation (1 variable);
- HP steam drum \( \Delta T_{Drum} \), which is the difference between subcooled water saturation temperature and its stream \( T \). This defines subcooled water \( T \) for HP steam generation (1 variable);
- HP superheaters OUT-stream temperatures (3 variables);
- HP steam independent mass flows in the 'cold side' superstructure (8 variables);
- Integer variables '\( z \)' for HP steam superheaters (3 variables);
- Gas turbine exhaust independent molar flows in the 'hot side' superstructure (15 variables).

\(^3\) except other independent molar flows fixed in the simulation at \( 1.0 \times 10^{-7} \text{ kmol/s} \).
8.2.1 Description of the solution

Using the ideal water/steam thermopack, the solution of this problem is described as follows:

- Running the MINLP_BB with initial TR=30 and a smoothing parameter $\epsilon = 2.0 \times 10^{-4}$ the algorithm converged in the first NLP subproblem (finding the required integer feasible solution). The MINLP_BB solver reported convergence as shown in Table 8.1.

Table 8.2 gives the optimised values for some of the free variables that were fixed when we solved a simulation problem for providing a starting guess for this synthesis model.

Table 8.1: Results from the synthesis of HP steam superheaters.

<table>
<thead>
<tr>
<th>Results from MINLP_BB solver</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
<td>74.55</td>
</tr>
<tr>
<td>Number of NLPs solved:</td>
<td>1</td>
</tr>
<tr>
<td>Number of NLPs generated:</td>
<td>1</td>
</tr>
<tr>
<td>Total number of QPs solved:</td>
<td>31</td>
</tr>
<tr>
<td>... of which infeasible QPs:</td>
<td>0</td>
</tr>
<tr>
<td>Average number of QPs solved per NLP:</td>
<td>31.00</td>
</tr>
<tr>
<td>Average CPU time per NLPs (s):</td>
<td>74.55</td>
</tr>
<tr>
<td>Function evaluations:</td>
<td>29</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
<td>30</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
<td>14</td>
</tr>
<tr>
<td>Final value $f(x^*)$, [k$/year$]:</td>
<td>-2,461.378</td>
</tr>
</tbody>
</table>

Table 8.2: Optimised values for some free variables in the synthesis of HP steam superheaters (here 'shtr' means superheater, see also Fig. 8.1).

<table>
<thead>
<tr>
<th>Stream or unit</th>
<th>simulation fixed value</th>
<th>optimised value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water for steam generation $F$, [kg/s]:</td>
<td>6.61</td>
<td>12.346</td>
<td>6.0 - 31.0</td>
</tr>
<tr>
<td>HP steam drum $\Delta T_{\text{Drum}}$, [°C]:</td>
<td>3.0</td>
<td>2.0</td>
<td>2.0 - 50.0</td>
</tr>
<tr>
<td>HP steam in:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HP shtr 1 OUT-stream $T$, [°C]:</td>
<td>450.0</td>
<td>400.0</td>
<td>400.0 - 500.0</td>
</tr>
<tr>
<td>HP shtr 2 OUT-stream $T$, [°C]:</td>
<td>403.0</td>
<td>259.7</td>
<td>0.0 - 500.0</td>
</tr>
<tr>
<td>HP shtr 3 OUT-stream $T$, [°C]:</td>
<td>350.0</td>
<td>259.7</td>
<td>0.0 - 500.0</td>
</tr>
<tr>
<td>'z' for superheater 1: (optimum $Q = 3.468 \times 10^3$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>'z' for superheater 2: (optimum $Q = 0$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>'z' for superheater 3 (optimum $Q = 0$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
</tbody>
</table>
Description of synthesised structure

- The synthesised solution contains only the HP evaporator and one of the HP superheaters as shown in Fig. 8.2.

- In the synthesised solution superheater 'shtX' 2 and 3 (Fig. 8.1) have $z = 1$ and $Q = 0$. Therefore, they are effectively absent in the solution.

A few important operating variables obtained as a result of the optimised solution from the MINLP.BB solver are shown in Table 8.3. Note that the optimised profit (kS 2,461.378/year) is substantially different from the starting value. In addition, stack temperature and HP boiler minimum approach temperature were moved well below from their starting points. This shows that the model predicts reasonable results, because we obtained substantial improvement of the objective function associated with the predicted optimal structure.

<table>
<thead>
<tr>
<th>concept</th>
<th>optimised value</th>
<th>simulation design value</th>
</tr>
</thead>
<tbody>
<tr>
<td>O.F.: Total cost, [k$/year]:</td>
<td>-2,461.378</td>
<td>524.467</td>
</tr>
<tr>
<td>Stack temperature, [°C]:</td>
<td>264.2</td>
<td>357.2</td>
</tr>
<tr>
<td>HP Boiler min. approach $\Delta T$, [°C]:</td>
<td>5.0</td>
<td>97.8</td>
</tr>
</tbody>
</table>
8.3 Synthesis of HR exchangers in a double pressure steam combined cycle

This is the most complex problem solved in the research and consists of synthesising a network of waste heat recovery (HR) exchangers in a double pressure steam combined cycle. This model was solved as continuous optimisation problem in Chapter 7, Section 7.7.2.

The HR exchangers to synthesise are part of a HRSG whose source of heat is the exhaust from a commercial gas turbine that produces electricity. Steam is produced at two pressure levels, LP steam for deaeration purposes and HP superheated steam for producing additional power from steam turbines. The flowsheet was given in Chapter 7, Section 7.7 and is shown again here in Fig. 8.3 for easy reference.

The synthesis alternatives are included in a hyperstructure which contains 1 LP evaporator, 1 HP evaporator, up to 3 HP economisers and up to 3 HP superheaters, and considers all the possibilities for mixing/splitting and recycling of both the hot stream (gas turbine exhaust) and the cold stream (water/steam streams). In addition, in the synthesis model HR exchangers can potentially be in series or in parallel with respect to one another. A detailed explanation of how we constructed the hyperstructure for this model is given in Chapter 3, Section 3.5.3. In Fig. 8.3, economisers 1-3 are referred to as ‘HP EC1’ - ‘HP EC3’, while superheaters as ‘HP shtr 1’ - ‘HP shtr 3’.

The synthesis problem is given by minimising the total plant cost, as explained in Chapter 7, Section 7.7.2, subject to the MINLP model and bounds on variables.

The construction of the whole model in FMS represents a difficult task. For doing this, we constructed individual plant sections, which were used to build the whole synthesis model, including (see also Fig 8.4):

- The gas turbine.

- The hyperstructure model (as explained in Chapter 3, Section 3.5.3) for waste heat recovery exchangers built from: mixers and splitters for hot and cold streams, HR exchangers models and logical constraints.

- The steam system involving 2 steam turbines, an air-cooled condenser, a deaerator, pumps, valves and mixers/splitters.
Figure 8.3: Flowsheet for the synthesis of heat recovery exchangers in a combined cycle.

*Details of hot side superstructure are given in Chapter 3, Section 3.5.3 and in Fig. 3.5.
Figure 8.4: Models in FMS for the synthesis of waste heat exchangers in a combined cycle with two steam pressure levels.
The model defined in FMS contains 3042 variables and 2139 constraints. For this synthesis model we have 98 free variables and 805 specifications.

Thus, the synthesis problem for finding the optimal number and location of heat recovery (HR) exchangers in a combined cycle considers:

- O.F. = minimise annualised capital and operating cost combined with a revenue from selling electricity obtained from gas and steam turbines (given by our so called 'general economic objective function');
- the plant model including a hyperstructure for synthesis of HR exchangers;
- water/steam streams ideal thermopack;
- 1 LP evaporator (fixed integer variable \( z = 1 \));
- 1 HP evaporator (fixed \( z = 1 \));
- up to 3 HP superheaters (with free integer variables);
- up to 3 HP economisers (with free integer variables);
- a total of 98 free variables including independent mass/molar flows and independent temperatures in the hyperstructure, details were given in Chapter 7, Section 7.7.2.

### 8.3.1 Model solution

Using the MINLP_BB solver the successful run consisted of:

1. Starting with smoothing parameter \( \epsilon = 2.0 \times 10^{-4} \) the MINLP_BB finished in 5 QPs solved with a termination code "ifail=1" (a Kuhn-Tucker point of the feasibility problem).
2. Taking the variable values from there, we ran again the MINLP_BB solver using \( \epsilon = 1.0 \times 10^{-4} \).

Branching iterations were (see also Fig. 8.5):

A In 'problem 0' (or the 1st NLP) we found a not integer feasible solution with \( O.F. = 4539.381 \), branch on \( z = 0.6994 \) (for economiser 3). There the MINLP_BB solver intro-
duced 2 new problems: ‘**problem 1**’ with \( z = 1 \) for economiser 3 and ‘**problem 2**’ with \( z = 0 \) for economiser 3.

**B** The MINLP.BB solver found an integer feasible solution for ‘**problem 1**’ with \( O.F. = 4539.381 \), being this the solution to the MINLP problem, so we do not need to solve ‘**problem 2**’.

The MINLP.BB solver reported convergence parameters as shown in Table 8.4.

Table 8.5 shows some relevant optimised variables compared with their corresponding starting point values that were previously fixed to solve a simulation problem.

**solution description**

- The optimal superheated steam temperature is \( T = 436.0 °C \).

- As shown in Fig. 8.6 the synthesised structure implies the presence of the following HR exchangers:

![Figure 8.5: Branching iterations for HR exchangers synthesis problem in a combined cycle.](image)
- 1 LP evaporator, 1 HP evaporator;
- HP economiser 3 (‘HP EC3’ in Fig. 8.3) was selected among the three potential economisers.
- HP superheater 1 (‘HP shtr 1’ in Fig. 8.3) was selected among the three potential superheaters.

Table 8.4: HR exchangers synthesis for a double pressure steam combined cycle (water/steam ideal thermopack).

<table>
<thead>
<tr>
<th>Results from MINLP_BB solver</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s):</td>
</tr>
<tr>
<td>Number of NLPs solved:</td>
</tr>
<tr>
<td>Number of NLPs generated:</td>
</tr>
<tr>
<td>Total number of QPs solved:</td>
</tr>
<tr>
<td>... of which infeasible QPs:</td>
</tr>
<tr>
<td>Average No. of QPs solved per NLP:</td>
</tr>
<tr>
<td>Average CPU time for NLPs (s):</td>
</tr>
<tr>
<td>Function evaluations:</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
</tr>
<tr>
<td>Final value $f(x^*)$, [k$/year$]:</td>
</tr>
</tbody>
</table>

Table 8.5: Optimised values for some free variables in the cost minimisation of the synthesis model for a double pressure steam combined cycle.

<table>
<thead>
<tr>
<th>Stream or unit</th>
<th>simulation fixed value</th>
<th>optimised value</th>
<th>bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deaerated water $T_1$, [°C]:</td>
<td>57.7</td>
<td>54.78</td>
<td>44.0 - 200.0</td>
</tr>
<tr>
<td>Deaerator operating $P_1$, [MPa]:</td>
<td>0.0179</td>
<td>0.0175</td>
<td>0.015 - 3.0</td>
</tr>
<tr>
<td>LP steam generated $P_2$, [MPa]:</td>
<td>0.0198</td>
<td>0.0176</td>
<td>0.015 - 3.0</td>
</tr>
<tr>
<td>HP Turbine OUT-stream $P_3$, [MPa]:</td>
<td>0.331</td>
<td>0.155</td>
<td>0.07 - 12.5</td>
</tr>
<tr>
<td>LP Turbine OUT-stream $P_4$, [MPa]:</td>
<td>0.01235</td>
<td>0.01278</td>
<td>0.001 - 12.5</td>
</tr>
<tr>
<td>HP steam drum $\Delta T_{Drum}$, [°C]:</td>
<td>3.0</td>
<td>2.0</td>
<td>2.0 - 50.0</td>
</tr>
<tr>
<td>HP shtr 1 OUT-stream $T_5$, [°C]:</td>
<td>450.0</td>
<td>436.0</td>
<td>150.0 - 500.0</td>
</tr>
<tr>
<td>HP shtr 2 OUT-stream $T_6$, [°C]:</td>
<td>403.0</td>
<td>259.4</td>
<td>150.0 - 500.0</td>
</tr>
<tr>
<td>HP shtr 3 OUT-stream $T_7$, [°C]:</td>
<td>350.0</td>
<td>436.0</td>
<td>150.0 - 500.0</td>
</tr>
<tr>
<td>$z_1$ for superheater 1 (optimum $Q = 4.213 \times 10^3$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>$z_1$ for superheater 2 (optimum $Q = 0$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>$z_1$ for superheater 3 (optimum $Q = 0$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>$z_1$ for economiser 1 (optimum $Q = 1.69 \times 10^{-5}$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>$z_1$ for economiser 2 (optimum $Q = 3.99 \times 10^{-8}$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
<tr>
<td>$z_1$ for economiser 3 (optimum $Q = 10.147 \times 10^3$ kW):</td>
<td>1</td>
<td>1</td>
<td>0 - 1</td>
</tr>
</tbody>
</table>
In the synthesised solution economisers 1 and 2 have \( z = 1 \), but with small heat loads \( Q = 1.69 \times 10^{-5} \text{ kW} \) and \( Q = 3.99 \times 10^{-8} \text{ kW} \) respectively and no sensible change in temperature of water and exhaust gas across this equipments. Thus these HR exchangers essentially do not exist in the optimal structure for engineering purposes.

In the synthesised solution superheaters 2 and 3 have \( z = 1 \), but with heat load \( Q = 0.0 \text{ kW} \), thus these superheaters do not exist in the optimal structure.

In Table 8.6 are shown some relevant operating variables compared with their corresponding starting guess values.
8.3.2 Synthesised structure simulated with filterSQP code

Now, after we solved the synthesis model with the water/steam ideal thermopack and found the optimal structure, we use the rigorous thermopack and the filterSQP code with two objectives in mind: a) to compare the results from the rigorous against the ideal thermopacks for the same structure; and b) to compare with the optimal synthesis obtained for this model using the filterSQP code in Chapter 7, Section 7.7.2.

From the simulation using the filterSQP we may compare objective function values and other relevant parameters throughout the system given by the two thermopacks.

Thus we construct the model in FMS for the optimal structure using the rigorous water/steam thermopack (presented in Appendix A). We provide relevant fixed variables obtained from the solution with ideal thermopack to the new model as to have zero free variables and no redundant equations (checked with the EA). However the fully constrained model for the rigorous thermopack having fixed variables from the ideal thermopack solution prevented filterSQP to converge the model. This is because the two thermopacks give temperatures, enthalpies and other variables throughout the plant which may be very different (i.e. the problem was 'ideally' constrained so the model with accurate thermopack could not be solved).

For a successful ‘simulation’ using filterSQP and rigorous thermopack, the following few variables were left free: Deaerator OUT-stream temperature, mass flow to LP steam turbine and LP turbine outlet pressure. At solution with filterSQP these variables got similar values as
from the simplified thermopack. The maximum difference between them is 3.4%. FilterSQP solution for the simulation of the optimal structure is shown in Table 8.7.

### 8.3.3 Comparing the solutions from the two thermopacks

In Table 8.8 some variable values for the optimal structure are compared when the combined cycle model is solved using the simplified and the accurate water/steam thermopacks. The

<table>
<thead>
<tr>
<th>Table 8.7: Simulation of the synthesised structure using filterSQP and the rigorous thermopack.</th>
</tr>
</thead>
<tbody>
<tr>
<td>filterSQP</td>
</tr>
<tr>
<td>Total CPU time (s):</td>
</tr>
<tr>
<td>Iterations:</td>
</tr>
<tr>
<td>... of which iterations in inf. NLP:</td>
</tr>
<tr>
<td>QP problems solved:</td>
</tr>
<tr>
<td>Total number of QP pivots:</td>
</tr>
<tr>
<td>Function evaluations:</td>
</tr>
<tr>
<td>Constraint evaluations:</td>
</tr>
<tr>
<td>Gradient evaluations:</td>
</tr>
<tr>
<td>Final value ( f(x^*) ), [k$/year]</td>
</tr>
<tr>
<td>Initial/Final TR radius:</td>
</tr>
<tr>
<td>Dimension of null space:</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 8.8: Relevant operating variables for the synthesis problem of a double pressure steam combined cycle (comparing water/steam thermopacks).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermopack:</td>
</tr>
<tr>
<td>O.F.: Total cost, [k$ / yr.]</td>
</tr>
<tr>
<td>Optimised value:</td>
</tr>
<tr>
<td>Plant Thermal efficiency</td>
</tr>
<tr>
<td>Deaerated water ( T ), [°C]:</td>
</tr>
<tr>
<td>LP Turbine IN-stream ( F ), [kg/s]:</td>
</tr>
<tr>
<td>LP Turbine OUT-stream ( P ), [MPa]:</td>
</tr>
<tr>
<td>LP steam turbine ( W ), [kW]:</td>
</tr>
<tr>
<td>HP steam turbine ( W ), [kW]:</td>
</tr>
<tr>
<td>Air-cooled condenser ( Q ), [kW]:</td>
</tr>
<tr>
<td>HP Superheater ( Q ), [kW]:</td>
</tr>
<tr>
<td>HP Boiler ( Q ), [kW]:</td>
</tr>
<tr>
<td>HP Economiser ( Q ), [kW]:</td>
</tr>
<tr>
<td>LP Boiler ( Q ), [kW]:</td>
</tr>
<tr>
<td>Air-cooled condenser ( A ), [m²]:</td>
</tr>
<tr>
<td>HP Superheater ( A ), [m²]:</td>
</tr>
<tr>
<td>HP Boiler ( A ), [m²]:</td>
</tr>
<tr>
<td>HP Economiser ( A ), [m²]:</td>
</tr>
<tr>
<td>LP Boiler ( A ), [m²]:</td>
</tr>
<tr>
<td>stack temperature, [°C]:</td>
</tr>
</tbody>
</table>
difference between variable values can be as large as about 34% for heat loads and heat transfer areas. This is an indication of how important it is to use a rigorous water steam thermopack in the solution of utility systems problems.

8.4 Analysis of results from the synthesis examples

The MINLP.BB solver failed to solve our synthesis models having the rigorous water/steam streams thermopack. The software package reported the trust region (TR) value decreasing below the solver tolerance, as the optimisation proceeded. This was observed generally in the branching iterations i.e. in NLPs other than the first NLP relaxation. Possible reasons include:

- The non-convex nature of the rigorous thermopack may produce difficulties for the robustness of the MINLP.BB solver especially in branching iterations (in the NLP subproblems).
- Warm-guess and scale factors provided for a starting structure may not always help the convergence process of the solver. In particular when some streams (and units) go to zero or to their lower bound (e.g. $1.0 \times 10^{-7}$ kmol/s for gas turbine exhaust streams), thus during the synthesis solution the problem may become badly scaled affecting the robustness of the MINLP.BB optimiser.
- The non-smooth function (for the $q$ vs. $\phi$ relationship) in the water/steam model (explained in Chapter 3, Section 3.1.1) proved to work very efficiently when we solved EO simulation and NLP optimisation problems. However, for our synthesis problems with many free variables (from 31 to 98 in our examples), the use of non-smooth functions in the model may also affect the MINLP.BB solver robustness.

For successful solution of our synthesis problems, we used a strategy outlined in Section 8.1.2. This involves the use of an ideal water/steam thermopack and interactive use of a smoothed parameter, $\epsilon$.

For the synthesis example presented in Section 8.2, using $\epsilon = 2.0 \times 10^{-4}$ the MINLP.BB solver found, in the first NLP subproblem, an $O.F. = k$ \$/\text{year} = 2,461.378$ \$/\text{year}$. This provided the optimal structure since we found there an integer feasible solution.

$^{4}$ Is negative because we minimise our objective function which in turn was to maximise profit.
From the solution of the largest MINLP model using the filterSQP (presented in Chapter 7, Section 7.7.2) we saw there that the optimised annual cost is k$4,575.006. In this chapter (Section 8.3), we solved this MINLP model using the MINLP.BB solver and the ideal thermopack. Then using the synthesised structure (being the same found for this problem in Chapter 7, Section 7.7.2) and the rigorous thermopack we simulate the optimal structure using the filter-SQP code, this produced an annualised cost of k$ 4,597.083/year. The difference between the two objective function values is because, for this largest synthesis model solved in Section 8.3, we have not obtained simultaneously structural and parameter optimisation of the MINLP model using the MINLP.BB solver. Instead, we solved the synthesis model first using the ideal thermopack and then using the rigorous thermopack we compare the results from the two.

A comparison between the parameters given for the optimal structure using the ideal and the rigorous thermopacks gave an indication of the importance of using our rigorous thermopack in utility systems problems.

In our synthesised structures we observe that HR exchangers with heat load $Q \approx 0$ kW (or exactly zero) did not necessarily have an integer variable $z = 0$. This is because our model did not enforce such condition, but still provides the engineer with the optimal solution. The implication $Q = 0 \Rightarrow z = 0$ was not needed from the cost minimisation point of view as long as we minimised our objective function.

It is more desirable to adjust the model to state that for a given HR exchanger with $Q = 0$ the integer variable should be $z = 0$, especially for more complex synthesis problems, to fully exploit the existence of integer variables. This task may not be too difficult to implement.

We were able to obtain zero heat transfer area $A$, and consequently zero cost for non-optimal HR exchangers thanks to our smoothed cost functions. Original cost models for HR exchangers (and other units) have similar ‘mathematical form’ e.g. for waste heat evaporator is expressed as (Wells and Rose, 1986):

$$C = 3.3 \ A^{0.5}$$

where $C$ is the HR exchanger cost in k$ and $A$ is the heat transfer area in m$^2$. Clearly, the cost function as such, cannot be used in mathematical optimisation since it produces infinite derivatives as $A \rightarrow 0$. Our implementation of smoothing cost functions (explained in Chapter 3, Section 3.4.2) provides continuous and differentiable cost function at any $A$ value (including zero area). Thus, we could use them successfully to solve our synthesis and optimisation problems.
It is worth to note that, using smoothed cost functions we could successfully solve the largest synthesis model (with the accurate water/steam thermopack), as continuous NLP optimisation problem (Chapter 7, Section 7.7.2) in a more robust manner than with the MINLP.BB solver (solution shown in Section 8.3). It would be better to be able to solve the synthesis model with rigorous thermopack and the MINLP.BB solver, especially for problems with a larger number of integer variables (we solved synthesis models with up to 8).

Our synthesis model predicts quite well which HR exchangers should not be present in the optimal HRSG structure within the context of complete CHP systems. This was demonstrated more effectively using the rigorous water/steam thermopack and the filterSQP code alone. The use of ideal thermopack and MINLP.BB solver for synthesis problems with many more integer variables (e.g. considering 4-5 steam pressure levels and reheating) will probably be the better option to find the optimal structure, especially if the use of rigorous thermopack presents strong convergence difficulties.
Chapter 9

Conclusions and further work

This chapter presents the conclusions drawn from this research project on synthesis and optimisation of large-scale utility systems. As mentioned before the project has special relevance to combined heat and power (CHP) systems, where heat and power are produced from the same primary energy source, in our case, natural gas.

CHP systems are used to supply heat and power to industrial processes or to the utility grid and are described by highly integrated processes with a multi-loop nature where material, energy, and information may be recycled. In our systems in study we may have gas and steam turbines, steam generators (conventional or heat recovery steam generators, HRSG), pumps, condensers and other auxiliaries. The optimal combination of operating conditions and units arrangement is a complex problem that we proposed to study in an equation-oriented (EO) approach, where modelling equations are solved simultaneously.

For this research we have proposed EO models for process streams and unit operations relevant in utility systems, we then solved a number of simulation, optimisation and two synthesis problems. The size of our optimisation and synthesis problems range from about 100 to more than 3,000 variables. Section 9.1 presents concluding remarks on the main areas covered in this project while Section 9.2 shows the recommendations for future work.

9.1 Conclusions

We present conclusions for each of the main activities developed in this project:
○ **Equation oriented models** We have contributed with an extensive set of equation-oriented (EO) mathematical models for process streams and unit operations relevant to CHP systems. Models are a mixture of rigorous (for water/steam and air process streams) and realistic approximations (e.g. for gas turbines, waste heat exchangers, deaerator, etc.). The models are given by an independent set of algebraic equations (most of them non-linear) which are twice-continuously differentiable and can be solved simultaneously, stand-alone or in a network describing complete utility systems up to industrial size dimensions. For these models we have obtained 1st and 2nd partial derivative information with the aim of solving complex EO simulation, NLP optimisation and MINLP synthesis problems. Along with these models we proposed (taken data from the open literature) fixed and operating costs functions used in solving economic optimisation problems.

The water/steam stream model includes a non-smooth function between stream vapour fraction and quality. When solving optimisation problems, smoothing techniques in the model were necessary.

Stream and unit operations models include a set of variables which provide useful information for streams/units, for application in other plant sections (e.g. stream entropy for turbines) and that may be applied for further extension of models as required.

Our proposed models include a MINLP model for the synthesis of heat recovery (HR) exchangers in a HRSG which is part of a combined cycle (with gas and steam turbines) or of a cogeneration plant (where heat and power are produced).

We fully tested and demonstrated the very efficient applicability of our models in solving complex EO simulation and NLP optimisation problems.

The MINLP synthesis model using our rigorous water/steam streams model was not as robust as expected, perhaps due to:

- the many free variables (up to 98);
- the difficulty to provide a well scaled problem (where variables are of the same order of magnitude and equations and partial derivatives are also scaled) which in synthesis problems proved to be hard to set (except at the starting guess), since some streams and units may become 'non-present' while the MINLP solver finds the optimal structure; and

- the non-convex nature of models, in particular the rigorous water/steam stream's.

○ **Simulation problems**

In order to test both our proposed models and a new equation oriented modelling system, called FMS (Mitchell and Morton, 1996), we solved a number of EO simulation problems.
These include from single process streams and unit operations up to complete utility systems, including a cogeneration plant currently in operation (Gator-Power, 1994). Size of simulation models goes up to 3,022 variables and equations.

FMS has linked a set of tools for solving EO simulation problems including an equation analyser, EA (Morton and Collingwood, 1998) to check for the existence of redundant equations and free variables and a sparse Nonlinear Algebraic Equations (NLAE) solver (Morton, 1997). Our individual models were used to construct up to whole CHP systems models thanks to the capabilities of FMS.

The Flexible Modelling System (FMS) was used successfully to build complex models, which were analysed for correct formulation by the EA and solved by the sparse NLAE solver.

The Equation Analyser (EA) tool proved effective in assessing the proper model definition by identifying free variables and redundant equations in a given model.

In addition the sparse NLAE solver was extensively tested and advantage was taken of its features, such as a trust region (TR) and reordering strategies, for the successful simulation of the example problems.

For solving complex units and plant simulation models (e.g. for a commercial gas turbine and for whole utility systems) we proposed a strategy of supplying converged solutions to subsections which in turn were used as starting guess for larger models.

The effectiveness of this framework for simulating cogeneration plants using natural gas as fuel was demonstrated by solving a large set of problems. Perhaps the most relevant is the model of a real plant which accurately reproduced all the available key performance parameters like heat loads, water/steam pressures and temperatures, the gas turbine power produced and exhaust gas mass flow and distribution of temperatures throughout the plant.

In EO simulation problems the number of equations equals the number of variables (after proper specification of degrees of freedom).

In solving our simulation models, we extensively tested and demonstrated the efficient applicability of the proposed models and the EO environment.

NLP optimisation problems

Passing from simulation to an optimisation problem requires some variables to be freed. Once we mastered our strategy for solving EO simulation models we easily provided warm-starting guesses for the efficient solution of large-scale NLP optimisation problems.
CHAPTER 9. CONCLUSIONS AND FURTHER WORK

Using sequential quadratic programming (SQP) methods we solved a number of NLP optimisation problems for utility systems. Early testing of models includes the solution of an optimisation problem for a CHP plant using a SQP method (Zoppke-Donaldson, 1995) which uses a 'tolerance-tube' to decide whether or not each step solved by a QP point approximation of the NLP is acceptable. The 'tolerance-tube' SQP method has one version which exploits the sparsity of Jacobian and Hessian information.

Later, using FMS along with an advanced NLP optimisation package called filterSQP (Fletcher and Leyffer, 1998) and having implemented a scaling procedure for optimisation models, we solved many NLP problems for energy and economic optimisation of utility systems.

For a small problem, with 130 variables, several computational experiments to show the effect of scaling the problem; the effect on using a dense vs. a sparse filterSQP versions; the 'shadow price' of the HP steam temperature by using the relevant Lagrange multipliers information; and the trust region size effect were presented. Those experiments allowed further assessment of the EO utility model and the use of the filterSQP optimiser.

Our strategy of supplying a warm-starting guess obtained by simulation, and that of providing scaled problems to the filterSQP, was used in the efficient solution of NLP optimisation problems.

Problems' size goes from about 100 to 3,042 variables. The number of free variables ranges from 4 to 98.

The overall results are very promising for the use of the proposed models, of the sparse filterSQP version that has proved to be a robust and efficient solver for large-scale industrial size optimisation problems.

MINLP synthesis problems

We proposed a MINLP synthesis model for obtaining the optimal number and position of HR exchangers in a HRSG in the context of combined cycle and cogeneration plants.

We presented the solution of two synthesis models: one for a cogeneration system supplying electric power and HP steam (with 1,167 variables, 31 being free variables); and another for a double pressure steam combined cycle with 3,042 variables including 98 decision variables.

With the use of our rigorous water/steam thermopack when solving the synthesis models, the MINLP_BB package (Leyffer, 1998) failed to converge. Possible reasons were given before. Thus we proposed a strategy for solving our large-scale MINLP synthesis problems consisting in using an ideal thermopack and interactively supplying the smoothing
parameter for the non-smooth equation in the water/steam model. We then got the solution from the MINLP_BB solver. Then using the optimised structure, we compared results from the ideal against the rigorous water/steam thermopacks.

With this strategy, the model and the MINLP_BB solver proved to give satisfactory synthesised solutions. However, for the optimal structure the comparison of results from the ideal and the rigorous thermopacks demonstrates the need to use the accurate water/steam thermopack to obtain a more effective parameter and structural optimisation.

For our largest model with 8 integer variables we were able to obtain the synthesised solution using the filterSQP alone thanks to the fact that we used smoothed cost functions for HR exchangers which were synthesised. Nevertheless for synthesis problems with many more integer variables, advantage of the MINLP_BB solver should be taken.

In our synthesised structure we identify non-optimal ‘non-existent’ HR exchangers by looking at their heat load value (zero or very close to zero, e.g. $1.0 \times 10^{-4}$ kW or less). This was because for those HR exchangers the integer variable $z$ was not forced to be zero, but remained as $z = 1$, resulting from the form of our cost model. These cost functions are already smoothed, so $z$ may not needed to be zero as long as the optimised objective function was found.

We believe that our synthesised structures provide a satisfactory answer for the synthesis problem we wanted to solve, but further refining of the MINLP model is needed to assure that a HR with zero heat load is associated with an integer variable equal to zero and also to promote the direct solution of the model, using the rigorous water/steam thermopack, with the MINLP_BB solver.

Finally, as overall conclusions we could say that the results shown in this thesis are very promising for the applicability of both the EO model and the EO infrastructure especially for simulation and NLP optimisation of real combined cycle and cogeneration plants. MINLP synthesis was not as robust as expected, but may be used as such in preliminary selection of HR exchangers in the context of whole utility systems.

### 9.2 Recommendations for further work

One of the key advantages of an EO approach is the flexibility to extend the level of detail of the modelling equations. Interesting areas for new research in the modelling aspects include:
○ Smooth water/steam model. Our experience showed that the use of smoothed equations in our water/steam model may be a source of concern for the efficient solution of synthesis models with the MINLP_BB solver. Our non-smooth equation for quality and vapour fraction in this model comes from the necessity of finding a suitable set of equations describing this type of stream regardless of physical phase. It would be desirable to implement a water/steam model without any non-smooth function describing liquid or vapour or mixture of phases to eliminate this potential source of concern.

○ Adding more process streams variables. Addition of some more process streams variables like viscosity and thermal conductivity would allow more complex and interesting facilities for problem solving in utility systems, including the calculation of pressure drops and heat transfer coefficients.

○ Modelling other important process streams in utility systems. Process stream models may be easily added for thermal oils used in ‘hot oil heating circuits’ for indirect heating, as these have a number of applications including waste heat recovery from gas turbines.

○ Modelling additional process units. Utility systems have a wide range of process units which may be added to our basic set of models. It would be desirable to have models for heat pumps, fresh water production plants (e.g. by multistage flash evaporation), for a wider range of commercial gas turbines to choose from and for unit operations of non-conventional energy sources (e.g. solar cells, fuel cells). In that way we may be able to find optimal combinations of traditional and alternative energy sources in utility systems.

○ Economic data. We constructed our fixed and operating cost functions from open literature information which may need to be refined to obtain more reliable solutions from the economic point of view. So we hope this work may be of interest for people in industry who may share more accurate data cost and may later be able to use our EO approach.

○ Unsteady state models. The inclusion of unsteady state balances represents an interesting area for research in large-scale utility systems.

Regarding simulation, optimisation and synthesis problems the following areas for new investigation are suggested:

○ Simulation problems. We solved EO simulation problems in a new modelling framework where FMS provides access to an equation analyser (EA) and to a sparse NLAE solver. From the many experiments done in this research, improvements on the modelling system may include the capability of FMS to set up a new model once a previous one has been
solved. This means that now after we solved a problem for e.g. a given plant, we cannot straight away set up a model for another plant, instead we have to ‘quit’ FMS and start again to set up another model. In this respect, we just learnt that a new version of FMS is now ready (Mitchell, 1999) and does not have the stated drawback.

In chapter 6 we suggested that, in particular for large-scale models the EA may be improved by doing only stage (1): *structural analysis*, to provide the information on redundant equations and free variables. When constructing new models, care should be taken to write models in the form:

\[
\text{OUTPUTS} - \text{INPUTS} = 0
\]

so the EA may effectively help the engineer in selecting degrees of freedom. In this research these were chosen by applying the user’s intuition and the EA was mostly used for checking correct model definition rather than for helping in the selection of degrees of freedom.

- **SQP optimisation.** In the NLP optimisation problems solved we observed robust and efficient performance from the sparse filterSQP version. It is suggested to solve larger utility systems (or in general Process Engineering) problems to explore at which point the filter-SQP sparse version may no longer be a robust solver due to problems size and then explore other techniques for large-scale optimisation, perhaps decomposition in conjunction with parallel computing.

- **Synthesis problems.** The proposed MINLP model has the ability (at least for the examples shown) to predict the synthesis of HR exchangers in a HRSG, but does not enforce that HR units with heat load of zero imply integer variable \( z = 0 \). The MINLP model should be refined to satisfy such a condition. This refinement and the implementation of the water/steam model without any non-smoothness may help the robustness of later experiments on the MINLP synthesis model using the MINLP-BB solver.

Further desirable experiments on the MINLP model include the consideration of more complex HRSG units including 3 and more pressure steam levels and reheating which are used in current design practice. With this approach these features may be fully explored and optimised in the light of modern optimisation techniques.

From our basic MINLP synthesis model a further extension to consider not only HR synthesis but additional units, e.g. steam turbines, may be desirable.
Appendix A

Rigorous water/steam thermopack

This thermopack involves rigorous functions for the several physical properties needed in our water/steam stream model described in Chapter 3, Section 3.1.1.

A.1 Water enthalpy, $h_L$

The temperature and pressure effect on enthalpy is given by (Smith and Van Ness, 1987),

$$ dh = \left( \frac{\partial h}{\partial T} \right)_P dT + \left( \frac{\partial h}{\partial P} \right)_T dP \quad (A.1) $$

where:

$$ \left( \frac{\partial h}{\partial T} \right)_P = C_P \quad (A.2) $$

As an accurate mathematical expression for saturated water enthalpy, $h_f$ is available (Irvine and Liley, 1984), the liquid specific heat, $C_{PL}$ may be obtained by using (A.2) with $h_f = h$. This is valid for $T_r$ below $\sim 0.8$ (Reid et al., 1987). $^1$ Such an expression for $h_f$ in [kJ/kg] is:

$$ h_f = H_{fc} \left[ A + B \left( \frac{T_{cr} - T}{T_{cr}} \right)^{1/3} + C \left( \frac{T_{cr} - T}{T_{cr}} \right)^{5/6} + D \left( \frac{T_{cr} - T}{T_{cr}} \right)^{7/8} \right. $$

$$ + E_1 \left( \frac{T_{cr} - T}{T_{cr}} \right)^4 + \left. E_2 \left( \frac{T_{cr} - T}{T_{cr}} \right)^5 + E_3 \left( \frac{T_{cr} - T}{T_{cr}} \right)^6 \right. $$

$$ + E_4 \left( \frac{T_{cr} - T}{T_{cr}} \right)^7 ] $$

$$ (A.3) $$

$^1$ $T_r = T/T_{cr}$ (reduced temperature) below $\sim 0.8$ covers any practical steam-water system in the liquid phase according to (Papoulias and Grossmann, 1983a), (Peterson and Mann, 1985), (Stacy et al., 1981).
where $T$ is the absolute temperature, $H_{fcr} = 2.0993 \times 10^3$, $T_{cr} = 647.3 K$ (water critical temperature). And $A, \ldots, D, E_i, \ldots, E_7$ have fixed numerical values (Irvine and Liley, 1984) presented in Table A.1.

For the pressure dependence, basic thermodynamic expressions give (Smith and Van Ness, 1987):

$$\left( \frac{\partial h}{\partial P} \right)_T = v_L (1 - \beta T) \tag{A.4}$$

where $\beta$ is the thermal coefficient of expansion defined by:

$$\beta = \frac{1}{v_L} \left( \frac{\partial v_L}{\partial T} \right)_P \tag{A.5}$$

and $v_L$ is the specific volume of the fluid.

For liquid water a method for compressed liquids is used to calculate specific volume (Reid et al., 1987):

$$v_L = v_s \left[ 1 - c \ln \left( \frac{\zeta + P}{\zeta + P_{sat}} \right) \right] \tag{A.6}$$

where $P$ is the pressure in [MPa] and the variables $v_s, c, \zeta$ are described below. $P_{sat}$ (the saturation pressure) is described in Section A.8.

### Table A.1: Constants for saturated liquid enthalpy, $h_f$. 

<table>
<thead>
<tr>
<th>Constant</th>
<th>$273.16 \leq T &lt; 300.0$ K</th>
<th>$300 \leq T &lt; 600.0$ K</th>
<th>$600.0 \leq T \leq 647.3$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>0.0</td>
<td>8.839230108 x10^{-1}</td>
<td>1.0</td>
</tr>
<tr>
<td>$B$</td>
<td>0.0</td>
<td>0.0</td>
<td>-4.41057805 x10^{-1}</td>
</tr>
<tr>
<td>$C$</td>
<td>0.0</td>
<td>0.0</td>
<td>-5.52255517</td>
</tr>
<tr>
<td>$D$</td>
<td>0.0</td>
<td>0.0</td>
<td>6.43994847</td>
</tr>
<tr>
<td>$E(1)$</td>
<td>6.24698837 x10^2</td>
<td>-2.67172935</td>
<td>-1.64578795</td>
</tr>
<tr>
<td>$E(2)$</td>
<td>-2.34385369 x10^3</td>
<td>6.22640035</td>
<td>-1.30574143</td>
</tr>
<tr>
<td>$E(3)$</td>
<td>-9.50812101 x10^3</td>
<td>-1.31789573 x10^1</td>
<td>0.0</td>
</tr>
<tr>
<td>$E(4)$</td>
<td>7.16287928 x10^4</td>
<td>-1.91322436</td>
<td>0.0</td>
</tr>
<tr>
<td>$E(5)$</td>
<td>-1.63535221 x10^5</td>
<td>6.87937653 x10^1</td>
<td>0.0</td>
</tr>
<tr>
<td>$E(6)$</td>
<td>1.66531093 x10^5</td>
<td>-1.24819906 x10^2</td>
<td>0.0</td>
</tr>
<tr>
<td>$E(7)$</td>
<td>-6.47854585 x10^4</td>
<td>7.21435404 x10^1</td>
<td>0.0</td>
</tr>
</tbody>
</table>
The saturated liquid volume, \( v_s \) in \([m^3/kg]\) is given by:

\[
v_s = v_{cr} \left[ AA + BB \left( \frac{T_{cr} - T}{T_{cr}} \right)^{1/3} + CC \left( \frac{T_{cr} - T}{T_{cr}} \right)^{5/6} + \right.
\]

\[
+ DD \left( \frac{T_{cr} - T}{T_{cr}} \right)^{7/8} + EE_1 \left( \frac{T_{cr} - T}{T_{cr}} \right) + EE_2 \left( \frac{T_{cr} - T}{T_{cr}} \right)^2 + 
\]

\[
+ EE_3 \left( \frac{T_{cr} - T}{T_{cr}} \right)^3 \frac{EE_4 \left( \frac{T_{cr} - T}{T_{cr}} \right)^4 + EE_5 \left( \frac{T_{cr} - T}{T_{cr}} \right)^5 +}{T_{cr}^4} 
\]

\[
+ EE_6 \left( \frac{T_{cr} - T}{T_{cr}} \right)^6 + EE_7 \left( \frac{T_{cr} - T}{T_{cr}} \right)^7 \right] 
\]

where \( v_{cr} = 3.155 \times 10^{-3} \), \( T_{cr} \) is the water critical temperature as mentioned before. \( AA, \ldots, DD, EE_1, \ldots, EE_7 \) have the fixed numerical values given in Table A.2 for the full subcooled liquid temperature range \((273.16 - 647.3 \text{ K})\) (Irvine and Liley, 1984).

Also:

\[
\frac{\zeta}{P_{cr}} = -1 + aa \left( 1 - \frac{T}{T_{cr}} \right)^{1/3} + bb \left( 1 - \frac{T}{T_{cr}} \right)^{2/3} + 
\]

\[
+ d \left( 1 - \frac{T}{T_{cr}} \right) e \left( 1 - \frac{T}{T_{cr}} \right)^{4/3} 
\]

\[
e = \exp(f + g \omega + h \omega^2) 
\]

\[
c = j + k \omega 
\]

Table A.2: Constants for saturated liquid volume, \( v_s \).

<table>
<thead>
<tr>
<th>Constant</th>
<th>( 273.16 \leq T \leq 647.3 \text{ K} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( AA )</td>
<td>1.0</td>
</tr>
<tr>
<td>( BB )</td>
<td>-1.9153882</td>
</tr>
<tr>
<td>( CC )</td>
<td>1.2015186 \times 10^1</td>
</tr>
<tr>
<td>( DD )</td>
<td>-7.8464025</td>
</tr>
<tr>
<td>( EE(1) )</td>
<td>-3.888614</td>
</tr>
<tr>
<td>( EE(2) )</td>
<td>2.0582238</td>
</tr>
<tr>
<td>( EE(3) )</td>
<td>-2.0829991</td>
</tr>
<tr>
<td>( EE(4) )</td>
<td>8.2180004 \times 10^{-1}</td>
</tr>
<tr>
<td>( EE(5) )</td>
<td>4.7549742 \times 10^{-1}</td>
</tr>
<tr>
<td>( EE(6) )</td>
<td>0.0</td>
</tr>
<tr>
<td>( EE(7) )</td>
<td>0.0</td>
</tr>
</tbody>
</table>
In the last three equations, the variables $P_{cr}$ (water critical pressure in MPa), $aa$, $bb$, $d$, $f$, $g$, $h$, $j$, $k$, and $\omega$ (the acentric factor) have constant values taken from (Reid et al., 1987) and shown in Table A.3.

Table A.3: Constants for equations A.8 - A.10.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{cr}$</td>
<td>$2.2089 \times 10^1$</td>
</tr>
<tr>
<td>$aa$</td>
<td>$-9.070217$</td>
</tr>
<tr>
<td>$bb$</td>
<td>$6.245326 \times 10^1$</td>
</tr>
<tr>
<td>$d$</td>
<td>$-1.351102 \times 10^2$</td>
</tr>
<tr>
<td>$f$</td>
<td>$4.79594$</td>
</tr>
<tr>
<td>$g$</td>
<td>$0.250047$</td>
</tr>
<tr>
<td>$h$</td>
<td>$1.14188$</td>
</tr>
<tr>
<td>$j$</td>
<td>$0.0861488$</td>
</tr>
<tr>
<td>$k$</td>
<td>$0.0344483$</td>
</tr>
<tr>
<td>$\omega$</td>
<td>$0.3852$</td>
</tr>
</tbody>
</table>

Now, from equation (A.1) and the above considerations our accurate liquid water enthalpy correlation was obtained from,

$$h_L(T, P) = \int_{P_o}^{P} C_{pL} dT + \int_{P_o}^{P} \left[ v_L - T \left( \frac{\partial v_L}{\partial T} \right)_P \right] dP$$

(A.11)

where $P_o = 0.000611$ MPa and $T_o = 273.16K$. The solution of integrals in the right hand side of the last equation as well as the partial derivative information were obtained using the program Maple V.

2 Water enthalpy changes obtained using our enthalpy function compared with the ones obtained from a commercial modular physical property package, PPDS (NEL and IChemE, 1981) are within an error of 0.3%.
APPENDIX A. RIGOROUS WATER/STEAM THERMOPACK

A.2 Superheated steam enthalpy, $h_V$

Obtained from,

$$h_V(T, P) = B_{hv}(1) + B_{hv}(2)P + B_{hv}(3)P^2 + \left( B_{hv}(4) + B_{hv}(5)P \right)$$

$$+ B_{hv}(6)P^2\right)T + \left( B_{hv}(7) + B_{hv}(8)P + B_{hv}(9)P^2 \right)T^2$$

$$- \left( B_{hv}(10) + B_{hv}(11)T_s + B_{hv}(12)T_s^2 + B_{hv}(13)T_s^3 \right.$$ \n
$$+ B_{hv}(14)T_s^4 \exp \left( \frac{T_s - T}{M} \right) \right) \quad (A.12)$$

where $T_s$ is the saturation temperature. $B_{hv}(1), \ldots, B_{hv}(14)$ and $M$, have numerical fixed values for the full temperature and pressure range for steam phase (300.0 - 1,040.0 K) and (0.001 - 20.0 MPa) respectively (Irvine and Liley, 1984). Values for those constants are in Table A.4.

A.3 Water entropy, $s_L$

Using basic thermodynamic relationships (Smith and Van Ness, 1987) and $C_p, v_L$ as detailed in Section A.1 we have,

$$s_L(T, P) = \int_{T_s}^{T} C_p \frac{dT}{T} - \int_{P_s}^{P} \left( \beta v_L \right) dP \quad (A.13)$$

Our entropy calculations then produced accurate results which were within 0.2% error compared to the ones obtained from PPDS (NEL and IChemE, 1981).

A.4 Superheated steam entropy, $s_V$

This is obtained from:

$$s_V(P, T) = A_{s0} + A_{s1}T + A_{s2}T^2 + A_{s3}T^3 + A_{s4}T^4 + B_{s1} \ln \left( 10P + B_{s2} \right)$$

$$- \left( C_{s0} + C_{s1}T + C_{s2}T_s^2 + C_{s3}T_s^3 + C_{s4}T_s^4 \right) \exp \left( \frac{T_s - T}{M} \right) \quad (A.14)$$

where $A_{s0}, \ldots, A_{s4}, B_{s1}, B_{s2}, C_{s0}, \ldots, C_{s4}$ and $M$, have numerical fixed values for the full temperature and pressure range for steam phase (300.0 - 1,040.0 K) and (0.001 - 20.0 MPa) respectively (Irvine and Liley, 1984). Values for these constants are shown in Table A.5.
Table A.4: Constants for superheated steam enthalpy, $h_V$.

<table>
<thead>
<tr>
<th>$B_{h_v}(n)$</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_{h_v}(1)$</td>
<td>$2.04121 \times 10^3$</td>
</tr>
<tr>
<td>$B_{h_v}(2)$</td>
<td>$-4.040021 \times 10^4$</td>
</tr>
<tr>
<td>$B_{h_v}(3)$</td>
<td>$-4.8095 \times 10^{-1}$</td>
</tr>
<tr>
<td>$B_{h_v}(4)$</td>
<td>$1.610693$</td>
</tr>
<tr>
<td>$B_{h_v}(5)$</td>
<td>$5.472051 \times 10^{-2}$</td>
</tr>
<tr>
<td>$B_{h_v}(6)$</td>
<td>$7.517537 \times 10^{-4}$</td>
</tr>
<tr>
<td>$B_{h_v}(7)$</td>
<td>$3.383117 \times 10^{-4}$</td>
</tr>
<tr>
<td>$B_{h_v}(8)$</td>
<td>$-1.975736 \times 10^{-5}$</td>
</tr>
<tr>
<td>$B_{h_v}(9)$</td>
<td>$-2.87409 \times 10^{-7}$</td>
</tr>
<tr>
<td>$B_{h_v}(10)$</td>
<td>$1.70782 \times 10^3$</td>
</tr>
<tr>
<td>$B_{h_v}(11)$</td>
<td>$-1.699419 \times 10^4$</td>
</tr>
<tr>
<td>$B_{h_v}(12)$</td>
<td>$6.2746295 \times 10^{-2}$</td>
</tr>
<tr>
<td>$B_{h_v}(13)$</td>
<td>$-1.0284259 \times 10^{-4}$</td>
</tr>
<tr>
<td>$B_{h_v}(14)$</td>
<td>$6.4561298 \times 10^{-8}$</td>
</tr>
<tr>
<td>$M$</td>
<td>$4.5 \times 10^1$</td>
</tr>
</tbody>
</table>

A.5 Superheated steam volume, $v_V$

In complex optimisation problems and in the synthesis models, the stream specific volume 'v' was added to the water/steam stream model described in Chapter 3, Section 3.1.1. This required the addition of the next constraint,

$$v = [\phi v_v(T, P) + (1 - \phi) v_L(T, P)] = 0$$  \hspace{1cm} (A.15)

which in turn uses the function given by equation (A.6) for the calculation of water specific volume. While for the superheated steam we have,

$$v_v(T, P) = \frac{RT}{P} - B_{v_v}(1) \exp(-B_{v_v}(2)T)$$

$$+ \frac{1}{10} \frac{B_{v_v}(3) - \exp(A_{v_v0} + A_{v_v1}T_s + A_{v_v2}T_s^2) \exp(T_s - T)}{T}$$  \hspace{1cm} (A.16)

where $B_{v_v}(1), \ldots, B_{v_v}(3), A_{v_v0}, \ldots, A_{v_v2}, R$ and $M$, have numerical fixed values for the full temperature and pressure range for steam phase (300.0 - 1,040.0 K) and (0.001 - 20.0 MPa) (Irvine and Liley, 1984). These constant values are given in in Table A.6.
Table A.5: Constants for superheated steam entropy, $s_v$.

<table>
<thead>
<tr>
<th>$A_{s0}$</th>
<th>4.6162961</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{s1}$</td>
<td>$1.039008 \times 10^{-2}$</td>
</tr>
<tr>
<td>$A_{s2}$</td>
<td>$-9.873085 \times 10^{-6}$</td>
</tr>
<tr>
<td>$A_{s3}$</td>
<td>$5.43411 \times 10^{-9}$</td>
</tr>
<tr>
<td>$A_{s4}$</td>
<td>$-1.170465 \times 10^{-12}$</td>
</tr>
<tr>
<td>$B_{s1}$</td>
<td>$-4.650306 \times 10^{-1}$</td>
</tr>
<tr>
<td>$B_{s2}$</td>
<td>$1.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>$C_{s0}$</td>
<td>1.777804</td>
</tr>
<tr>
<td>$C_{s1}$</td>
<td>$-1.802468 \times 10^{-2}$</td>
</tr>
<tr>
<td>$C_{s2}$</td>
<td>$6.854459 \times 10^{-5}$</td>
</tr>
<tr>
<td>$C_{s3}$</td>
<td>$-1.184424 \times 10^{-7}$</td>
</tr>
<tr>
<td>$C_{s4}$</td>
<td>$8.142201 \times 10^{-11}$</td>
</tr>
<tr>
<td>$M$</td>
<td>$8.5 \times 10^{1}$</td>
</tr>
</tbody>
</table>

Table A.6: Constants for superheated steam volume, $v_v$.

<table>
<thead>
<tr>
<th>$A_{vv0}$</th>
<th>$-3.741378$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{vv1}$</td>
<td>$-4.7838281 \times 10^{-3}$</td>
</tr>
<tr>
<td>$A_{vv2}$</td>
<td>$1.5923434 \times 10^{-5}$</td>
</tr>
<tr>
<td>$B_{vv(1)}$</td>
<td>$5.27993 \times 10^{-2}$</td>
</tr>
<tr>
<td>$B_{vv(2)}$</td>
<td>$3.75928 \times 10^{-3}$</td>
</tr>
<tr>
<td>$B_{vv(3)}$</td>
<td>$2.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>$R$</td>
<td>$4.61631 \times 10^{-4}$</td>
</tr>
<tr>
<td>$M$</td>
<td>$4.0 \times 10^{1}$</td>
</tr>
</tbody>
</table>
A.6 Enthalpy of saturated liquid, $h_f$

This is obtained by using equation (A.3) with $h_f(T_s)$, where $T_s$ is the saturation temperature.

A.7 Enthalpy of saturated vapour, $h_g$

This is calculated from (Irvine and Liley, 1984),

$$ h_g = H_{gcr} \left[ A + B \left( \frac{T_{cr} - T_s}{T_{cr}} \right)^{1/3} + C \left( \frac{T_{cr} - T_s}{T_{cr}} \right)^{5/6} + D \left( \frac{T_{cr} - T_s}{T_{cr}} \right)^{7/8} \right] + \frac{E_1 (T_{cr} - T_s)}{T_{cr}} + \frac{E_2 (T_{cr} - T_s)^2}{T_{cr}^2} + \frac{E_3 (T_{cr} - T_s)^3}{T_{cr}^3} + \frac{E_4 (T_{cr} - T_s)^4}{T_{cr}^4} + \frac{E_5 (T_{cr} - T_s)^5}{T_{cr}^5} + \frac{E_6 (T_{cr} - T_s)^6}{T_{cr}^6} + \frac{E_7 (T_{cr} - T_s)^7}{T_{cr}^7} \right] \quad (A.17) $$

where $H_{gcr} = 2.0993 \times 10^9$, the critical and saturation temperatures, $T_{cr}$, $T_s$ respectively are expressed in K. And $A$, $\ldots$, $D$, $E_1$, $\ldots$, $E_7$ have fixed numerical values (Irvine and Liley, 1984) given in Table A.7 for the full saturation temperature range (273.16 - 647.3 K).

A.8 Saturation pressure, $P_{sat}$

The saturation pressure, $P_{sat}$ in [MPa] is (Irvine and Liley, 1984):

$$ P_{sat} = \exp \left( Ant(0) + Ant(1)T + Ant(2)T^2 + Ant(3)T^3 + Ant(4)T^4 + \right. $$

$$ + Ant(5)T^5 + Ant(6)T^6 + Ant(7)T^7 + Ant(8)T^8 + $$

$$ \left. + Ant(9)T^9 + \frac{Ant(10)}{T - Ant(11)} \right) \quad (A.18) $$

where $Ant(0), \ldots, Ant(11)$ have fixed numerical values for the full subcooled liquid temperature range (273.16 - 647.3 K) (Irvine and Liley, 1984). Such values are given in Table A.8. Note that $P_{sat}(T)$ is used in the calculation of $v_L$ by equation (A.6) and is the function $P_{sat}(T_s)$ in the water/steam stream model (Chapter 3, Section 3.1.1.).

A.9 Extrapolation of subcooled liquid properties at temperature near and over the critical point

The simultaneous nature of our EO approach involves difficulties with the calculation of superheated streams at temperatures near or above the critical point. The constraint for water/steam
Table A.7: Constants for enthalpy of saturated vapour, $h_9$.

<table>
<thead>
<tr>
<th>Constant</th>
<th>$273.16 \leq T_s \leq 647.3$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>1.0</td>
</tr>
<tr>
<td>$B$</td>
<td>$4.57874342 \times 10^{-1}$</td>
</tr>
<tr>
<td>$C$</td>
<td>5.08441288</td>
</tr>
<tr>
<td>$D$</td>
<td>-1.48513244</td>
</tr>
<tr>
<td>$E(1)$</td>
<td>-4.81351884</td>
</tr>
<tr>
<td>$E(2)$</td>
<td>2.69411792</td>
</tr>
<tr>
<td>$E(3)$</td>
<td>-7.39064542</td>
</tr>
<tr>
<td>$E(4)$</td>
<td>$1.04961889 \times 10^1$</td>
</tr>
<tr>
<td>$E(5)$</td>
<td>-5.46840036</td>
</tr>
<tr>
<td>$E(6)$</td>
<td>0.0</td>
</tr>
<tr>
<td>$E(7)$</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Stream enthalpy considers liquid and vapour properties,

$$h - [\phi h_V (T, P) + (1 - \phi) h_L (T, P)] = 0 \quad (A.19)$$

For superheated streams the thermopack gets $h_L$ which eventually is multiplied by zero (or $1 - \phi$) in equation (A.19).

The problem is for streams where temperature is close or above the critical value $T_{cr} = 374.15$°C, where the liquid correlations are no longer valid nor physically meaningful.

The calculation of the liquid enthalpy $h_L$, saturated liquid volume $v_s$, liquid entropy $s_L$ and enthalpy of saturated vapour, $h_9$ involves the term,

$$\left( \frac{T_{cr} - T}{T_{cr}} \right)^m$$

which has an exponent ‘$m$’ with a fractional value, see e.g. equations (A.3), (A.7), (A.17). Thus for streams with $T > T_{cr}$ the term given by equation (A.20) cannot be calculated. To solve this problem we propose an approximation for liquid properties for temperatures near and above the critical point. Considering only the temperature effect, the extrapolated liquid enthalpy is,

$$h_{L,e} = C_1 + C_2 (T - T_{bound})$$

where $T_{bound} < T_{cr}$ and,

$$C_1 = \int_{T_o}^{T_{bound}} C_{PL} dT$$
Table A.8: Constants for saturation pressure, $P_{\text{sat}}$.

<table>
<thead>
<tr>
<th>Constant</th>
<th>$273.16 \leq T \leq 647.3$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Ant(0)$</td>
<td>$0.104592 \times 10^2$</td>
</tr>
<tr>
<td>$Ant(1)$</td>
<td>$-0.404897 \times 10^{-2}$</td>
</tr>
<tr>
<td>$Ant(2)$</td>
<td>$-0.417520 \times 10^{-4}$</td>
</tr>
<tr>
<td>$Ant(3)$</td>
<td>$0.368510 \times 10^{-6}$</td>
</tr>
<tr>
<td>$Ant(4)$</td>
<td>$-0.101520 \times 10^{-8}$</td>
</tr>
<tr>
<td>$Ant(5)$</td>
<td>$0.865310 \times 10^{-12}$</td>
</tr>
<tr>
<td>$Ant(6)$</td>
<td>$0.903668 \times 10^{-15}$</td>
</tr>
<tr>
<td>$Ant(7)$</td>
<td>$-0.199690 \times 10^{-17}$</td>
</tr>
<tr>
<td>$Ant(8)$</td>
<td>$0.779287 \times 10^{-21}$</td>
</tr>
<tr>
<td>$Ant(9)$</td>
<td>$0.191482 \times 10^{-24}$</td>
</tr>
<tr>
<td>$Ant(10)$</td>
<td>$-0.396806 \times 10^4$</td>
</tr>
<tr>
<td>$Ant(11)$</td>
<td>$0.395735 \times 10^2$</td>
</tr>
</tbody>
</table>

$C_2 = \frac{dC_1}{dT}$ at $T_{\text{bound}}$

A value of $T_{\text{bound}} = 342.25^\circ C$ (saturation pressure = 15.0 MPa) was selected for the linear extrapolation and $C_1 = 1610.0404$, $C_2 = 7.3279$ were obtained. Then for superheated streams such extrapolations for liquid properties indeed are multiplied by zero (or 1 - $\phi$) in the constraint calculation, e.g. equation (A.19).

Similar extrapolations were applied to saturated liquid volume, $v_3$, water specific volume $v_L$, liquid entropy $s_L$, enthalpy of saturated liquid, $h_f$ and enthalpy of saturated vapour, $h_g$.

The range of operation for water/steam streams in our CHP plants considers $P \leq 12.5$ MPa and $T \leq 570^\circ C$ according to current design practice (Dechamps, 1998). Since the saturation temperature $T_s$ at 12.5 MPa is 327.85 $^\circ C$, then we do not have any liquid stream at -or above- 327.85$^\circ C$. So, our rigorous thermopack is applied throughout all the operating conditions in the CHP plants considered.
A.10 Variable units for water/steam stream model

Units used for the variables of the proposed water/steam stream model are given in Table A.9. Names of these variables were mentioned in Chapter 3, Section 3.1.1.

Table A.9: Variable units for water/steam stream model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>kW</td>
</tr>
<tr>
<td>$h$</td>
<td>kJ/kg</td>
</tr>
<tr>
<td>$F$</td>
<td>kg/s</td>
</tr>
<tr>
<td>$\phi$</td>
<td>-</td>
</tr>
<tr>
<td>$T$</td>
<td>°C</td>
</tr>
<tr>
<td>$P$</td>
<td>MPa</td>
</tr>
<tr>
<td>$T_s$</td>
<td>°C</td>
</tr>
<tr>
<td>$s$</td>
<td>kJ/kg K</td>
</tr>
<tr>
<td>$q$</td>
<td>-</td>
</tr>
<tr>
<td>$h_f$</td>
<td>kJ/kg</td>
</tr>
<tr>
<td>$h_q$</td>
<td>kJ/kg</td>
</tr>
<tr>
<td>$v$</td>
<td>m$^3$/kg</td>
</tr>
</tbody>
</table>
Appendix B

Equation of state and thermopack for air

The Beattie-Bridgman equation of state can be solved explicitly for specific volume \( v \) as (Lee, 1954):

\[
v = \frac{R_{\text{air}} T}{P} + \frac{\alpha_0}{R_{\text{air}} T} + \frac{\beta_0 P}{R_{\text{air}}^2 T^2} + \frac{\gamma_0 P^2}{R_{\text{air}}^3 T^3}
\]

(B.1)

where,

\[
\alpha_0 = R_{\text{air}} T B_0 - A_o - \frac{R_{\text{air}} c}{T^2}
\]

\[
\beta_0 = -R_{\text{air}} T B_0 a + A_o a - \frac{R_{\text{air}} B_o c}{T^2}
\]

\[
\gamma_0 = \frac{R_{\text{air}} B_0 b c}{T^2}
\]

and the numerical constants for last equations are given in Table B.1.

By using equation (B.1) and \( C_p(T) \) from (Irvine and Liley, 1984), exact correlations for the air enthalpy, air entropy and their corresponding continuous partial derivatives were derived, using the following basic thermodynamic relationships (Smith and Van Ness, 1987):

\[
dh_a = C_v dT + \left[ v - T \left( \frac{\partial v}{\partial T} \right)_p \right] dP
\]

(B.2)

\[
ds_a = C_p \frac{dT}{T} - \left( \frac{\partial v}{\partial T} \right)_p dP
\]

(B.3)

Integration of equations (B.2) and (B.3) considers \( P_o = 0.1 \) MPa and \( T_o = 273.15K \)

The specific heat at constant pressure in [kJ/kg K] (Irvine and Liley, 1984) is given by,

\[
C_p(T) = \sum_{i=0}^{4} A(i) T^i
\]

(B.4)
where the values for $A(i)$ are given in Table B.2.

It should be mentioned that units for the variables in the air single component streams model are the same as for the water/steam model for common variables to both models: $H$, $h$, $F$, $T$, $P$, $s$, and $v$ (see Appendix A, Section A.10).

Table B.1: Constants in Beattie-Bridgman equation of state.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{\text{air}}$</td>
<td>0.2867 kJ/kg K</td>
</tr>
<tr>
<td>$A_0$</td>
<td>0.157110973 kJ m$^3$/kg$^2$</td>
</tr>
<tr>
<td>$B_0$</td>
<td>0.159048 $\times 10^{-2}$ m$^3$/kg</td>
</tr>
<tr>
<td>$a$</td>
<td>0.66738 $\times 10^{-3}$ m$^3$/kg</td>
</tr>
<tr>
<td>$b$</td>
<td>-0.3805 $\times 10^{-4}$ m$^3$/kg</td>
</tr>
<tr>
<td>$c$</td>
<td>1.49726804373 $\times 10^3$ m$^3$ K$^3$/kg</td>
</tr>
</tbody>
</table>

Table B.2: Constants in specific heat for air.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A(0)$</td>
<td>0.103409 $\times 10^1$</td>
</tr>
<tr>
<td>$A(1)$</td>
<td>-0.284887 $\times 10^{-3}$</td>
</tr>
<tr>
<td>$A(2)$</td>
<td>0.7816818 $\times 10^{-6}$</td>
</tr>
<tr>
<td>$A(3)$</td>
<td>-0.4970786 $\times 10^{-9}$</td>
</tr>
<tr>
<td>$A(4)$</td>
<td>0.1077024 $\times 10^{-12}$</td>
</tr>
</tbody>
</table>
Appendix C

Gas turbine streams thermopack

The calculations of enthalpy and entropy are given by ideal models:

\[ h_{\text{stream}}(P, T, y_i) = \sum y_i \int_{T_o}^{T} C_p \, dT \]  
\[ s_{\text{stream}}(P, T, y_i) = \sum y_i \int_{T_o}^{T} C_p \, \frac{dT}{T} - R \ln \frac{P}{P_o} - R \sum y_i \ln y_i \]  

The specific heat is given by polynomial expressions of the form,

\[ C_p = a_1 + a_2 \, x + a_3 \, x^2 + \cdots + a_7 \, x^6 \]  

where \( x = 1.0 \times 10^{-3} \, T \). Constant values for the different gas components considered in our EO model for streams in gas turbines are given in Appendix D, Tables D.1 and D.2 on pages 241-242. Values in these Tables give specific heat in [cal/mole K] and were transformed to [kJ/kmol K] within the actual thermopack. Specific heat correlations used here are valid for temperatures in the range (300.0 - 2,000.0 K). It should be mentioned that constant values for specific heat given in Tables D.1 and D.2 were obtained from (Prothero, 1969) for all the chemical species, except for \( C_2H_6 \) and \( n-C_5H_{12} \) for which specific heat was not available there, but obtained from ASPEN and then correlated to the form of equation (C.3).

C.1 Unit variables for gas turbine streams model

For this model variables have units as shown below. Names of these variables were mentioned in Chapter 3, Section 3.1.3.

<table>
<thead>
<tr>
<th>( H ), [kW]</th>
<th>( h ), [kJ/kmol]</th>
<th>( F ), [kmol/s]</th>
<th>( T ), [°C]</th>
<th>( P ), [MPa]</th>
<th>( s ), [kJ/kmol K]</th>
</tr>
</thead>
</table>
Appendix D

Equation oriented unit operations models

This appendix includes all the unit operations models used to model combined heat and power (CHP) systems in this thesis. Each model consists of material balances, energy balances, momentum balances and performance equations. The momentum balances allow there to be a pressure change but do not represent the momentum balances within the unit in any detail. The number of degrees of freedom obtained as number of variables minus number of equations is also included.

The unit models are an original contribution from this research except those for steam turbine (Morton and Rodríguez-Toral, 1997), mixer-splitter (single component streams), compressor, heater-cooler and valve (Morton, 1994a) which however are included here since all models shown in this appendix are used in modelling CHP systems.

D.1 Steam turbine

The unit is illustrated in Fig. D.1. The inlet and outlet streams have the variables and equations mentioned in Chapter 3, Section 3.1.1.

Material balance

\[ F_2 = F_1 \]  

(D.1)

Energy balance

\[ \eta_M (H_1 - H_2) = W \]  

(D.2)

where \( \eta_M \) (the mechanical efficiency) and the power output, \( W \), are regarded as local variables. The equation is written in this form to avoid division by \( \eta_M \) (Amarger et al., 1992).

Momentum balance / pressure change

\[ P_2 = P_1 - \Delta P \]  

(D.3)
where $\Delta P$ is the pressure drop through the steam turbine, regarded as a local variable.

**Performance equations**

The isentropic efficiency, $\eta_{iso}$ (another local variable), is defined by:

$$ h_1 - h_2 = \eta_{iso} (h_{1iso} - h_{iso}) \quad \text{(D.4)} $$

$h_{iso}$ is the outlet enthalpy for an ideal, isentropic turbine having the same pressure change as the real unit.

Four more equations are needed to define or correlate the isentropic outlet conditions:

$$ h_{iso} = \phi_{iso} h_V(T_{iso}, P_2) + (1 - \phi_{iso}) h_L(T_{iso}, P_2) \quad \text{(D.5)} $$

$$ s_1 = \phi_{iso} s_V(T_{iso}, P_2) + (1 - \phi_{iso}) s_L(T_{iso}, P_2) \quad \text{(D.6)} $$

$$ \phi_{iso} + a_{iso} q_{iso} = b_{iso} \quad \text{(D.7)} $$

$$ q_{iso} = \frac{(h_{92} - h_{iso})}{(h_{92} - h_{f2})} \quad \text{(D.8)} $$

where all the variables with subscript 'iso' refer to isentropic outlet conditions, and are regarded as local variables.

**Number of Degrees of Freedom**

The steam turbine should be responsible for the independent variables $F_2$, $P_2$, $h_2$ of the material stream OUT, the power output $W$ and also for some of the unit variables: $\Delta P$, $\eta_M$, $\eta_{iso}$, $h_{iso}$, $T_{iso}$, $\phi_{iso}$ and $q_{iso}$.

Of the unit variables, it is reasonable to regard the mechanical and isentropic efficiencies and the pressure drop as independent variables which determine the unit's performance. We have four equations to determine the four isentropic outlet variables (iso subscript) and the mass, energy and momentum balances respectively give $F_2$, $h_2$ (indirectly via the stream equation
\( H_2 = h_2 F_2 \) and \( P_2 \). Thus the number of degrees of freedom is,

\[
[(3 + 1 + 7)] - (3 + 1 + 4) = 11 - 8 = 3
\]

The model is sufficient to describe the unit given the 'natural' degrees of freedom: \( \Delta P, \eta_M \) and \( \eta_{iso} \).

### D.2 Gas turbine

This is a complex model consisting of three sections (see Fig. D.2):

- a compressor section;
- a combustion chamber with a pre-mixer for air and fuel (and steam in steam injected gas turbines (Tuzson, 1992)); and
- an expansion section.

The full EO model for a gas turbine includes the above subsections and the relationship between the work produced by the expansion section \( W_T \), the work required by the compressor section \( W_C \) and the net power output from the gas turbine \( W_{out} \). They are related to each other by,

\[
W_T \eta_{mt} = W_C + W_{out}
\]

where \( \eta_{mt} \) is the efficiency of mechanical transmission. Individual subsection models are below.

Variables and equations defining the gas turbine streams are given in Chapter 3, Section 3.1.3.

![Figure D.2: Sections and streams considered in the mathematical modelling of gas turbines.](image)
D.2.1 Compressor section

The compressor section of a gas turbine is modelled as shown in Fig. D.3. In this section air is compressed before it goes to the combustion chamber. Because combustion and equilibrium reactions are modelled in the combustion chamber, we need to use multicomponent stream models.

This unit operation model can be applied to general compressors (like the one needed to send fuel to the gas turbine combustor).

For a gas turbine the compressor section has 1 inlet and 1 outlet material streams. This section is driven by using power produced in the expansion section of the gas turbine.

Material balances

We use component mole balance equations for the stream IN (number 1) and the stream OUT (number 2). For $N$ components in a gas stream, we have $N$ component mole balance equations like:\footnote{In the component mole balance equations $i$ refers to the number of chemical species present in the stream, so $i = 1, \ldots, N$.}

$$F_2 y_{i,2} = F_1 y_{i,1} \quad (D.10)$$

where $F$ is the stream molar flow in $[\text{kmol/s}]$ and $y_{i}$ is the component mole fraction.

Energy balance

$$H_2 = H_1 + \eta_M W_C \quad (D.11)$$

where $\eta_M$ is the mechanical efficiency.

Momentum balance / pressure change
This equation relates inlet and outlet pressure,
\[ P_2 = P_1 r_{cp} \]  \hspace{1cm} (D.12)
where \( r_{cp} \) is the compressor pressure ratio.

**Performance equations**

One is for the isentropic efficiency,
\[ h_{iso} - h_1 = \eta_{iso}(h_2 - h_1) \]  \hspace{1cm} (D.13)
And two more equations for the isentropic outlet conditions,
\[ h_{iso} = h_{stream}(P_2, T_{iso}, y_i) \]  \hspace{1cm} (D.14)
\[ s_1 = s_{stream}(P_2, T_{iso}, y_i) \]  \hspace{1cm} (D.15)
where the subscript ‘iso’ refers to isentropic outlet conditions.

In equation (D.14) the function \( h_{stream} \) depends only on \( T \) and \( y_i \) in our current model, however it is written in a similar fashion as the \( s_{stream} \) just to be consistent in nomenclature and because in more rigorous models \( h_{stream} \) and \( s_{stream} \) both depend on \( P, T \) and \( y_i \).

**Number of Degrees of Freedom**

The compressor section should be responsible for the independent variables \( F_2, P_2, h_2, \) and \( N - 1 \) of the mole fractions \( y_i \) for the material stream OUT. And also of the unit variables: \( W_C, r_{cp}, \eta_M, \eta_{iso}, h_{iso} \) and \( T_{iso} \). So, the number of degrees of freedom is,
\[ [3 + (N - 1) + 6] - (N + 5) = 3 \]
Thus, the ‘natural’ degrees of freedom for the compressor section of a gas turbine are: \( r_{cp}, \eta_M \) and \( \eta_{iso} \).

**D.2.2 Combustion chamber**

In modelling the combustion chamber we consider first the mixing of air from the compressor section with fuel (and steam where appropriate), and then a combustion reaction section, see Fig. D.4. Models for both subsections describing the combustion chamber are given below.

**Model for the air/fuel mixer**

The air/fuel mixer (just before the combustion reactions take place) is modelled according to Fig. D.5.

**Material streams**

This mixer has 2 inlet and 1 outlet material streams. Here the local stream names are: AIR, FUEL, AIR/FUEL. While the local stream numbers are: 1, 2, 3.
Material balances

The component mole balance equations are:

\[
F_3 y_{i,3} = F_1 y_{i,1}
\]
\[
F_3 y_{j,3} = F_2 y_{j,2}
\]

where \( i = 1, \ldots, N_1 \); \( j = 1, \ldots, N_2 \). For \( N_1 \) components of stream 1 and \( N_2 \) components of stream 2, we have \( N_1 + N_2 \) component mole balance equations.

Energy balance

\[
H_3 = H_1 + H_2
\]

Momentum balances

\[
P_2 = P_1
\]
\[
P_3 = P_2
\]

Number of Degrees of Freedom

This mixer should be responsible for the independent variables: \( F, P \) and \( h + [(N_1 + N_2) - 1] \) of the mole fractions \( y_i \) for the outlet stream, 3. Therefore, the number of degrees of freedom
\[ ((N1 + N2 + 2) - (N1 + N2 + 1 + 2)) = -1 \]

This 'negative' degree of constraint occurs because the two inlet streams are forced to have the same pressure at the mixer. This means that the pressure of one of the two INLET streams e.g. fuel should be left unspecified, as is determined by the pressure at the mixer. Thus the mixer gives a degree of constraint for an upstream unit operation for the fuel stream. For example, it fixes the pressure raise of fuel going to the combustor through a fuel compressor.

**Model for the combustion reaction section**

The combustor model requires energy balance and reaction equilibrium equations to get the temperature and composition of the combustion products. The combustion products considered are: \( N_2, O_2, CO_2, H_2O \) as well as the the dissociation products obtained at high temperatures from these components and \( H_2 \).

When the products of a combustion reaction are at temperatures above 1,100 °C there is chemical dissociation of the constituent gases. Equations for the equilibrium composition must then be included in order to give the correct specific enthalpy and composition of the products stream (Rhine and Tucker, 1991). The model considers the use of natural gas with the first five alkanes (methane, ethane, propane, n-butane and n-pentane), identified as \( C_1, \ldots, C_5 \) respectively.

The combustion reactions for the combustion in air of the five hydrocarbons considered, are each described by an extent of reaction \( \epsilon_i, i = 1, \ldots, 5 \):

\[
\begin{align*}
CH_4 + 2O_2 & \rightarrow CO_2 + 2H_2O \\
C_2H_6 + \frac{7}{2}O_2 & \rightarrow 2CO_2 + 3H_2O \\
C_3H_8 + 5O_2 & \rightarrow 3CO_2 + 4H_2O \\
C_4H_{10} + \frac{13}{2}O_2 & \rightarrow 4CO_2 + 5H_2O \\
C_5H_{12} + 8O_2 & \rightarrow 5CO_2 + 6H_2O
\end{align*}
\]

**Equilibrium Reactions**

For high temperature combustion, we include dissociation reactions (Gaydon and Wolfhard, 1979) which are assumed to be at equilibrium. These have extents of reaction designated as \( \epsilon_i, i = 6, \ldots, 11 \) respectively for the 6 reactions:

\[
\begin{align*}
CO_2 & \rightleftharpoons CO + \frac{1}{2}O_2 \\
\frac{1}{2}N_2 + \frac{1}{2}O_2 & \rightleftharpoons NO \\
H_2O & \rightleftharpoons H_2 + \frac{1}{2}O_2 \\
H_2O & \rightleftharpoons \frac{1}{2}H_2 + OH \\
H_2 & \rightleftharpoons 2H \\
O_2 & \rightleftharpoons 2O
\end{align*}
\]

According to Fig. D.6, the combustion reaction section has 1 inlet and 1 outlet material streams. Local stream names: IN, OUT. Local stream numbers: 1, 2.
Material balance equations

Proposed for each of the components involved in the combustion and equilibrium reactions. They consider, where appropriate, the relevant extent of reaction $\epsilon_i$.

The mole balance for the fuel components in stream 1 (Fig. D.6) are given by:  

\begin{align*}
F_1 \ y_{C1,1} - \epsilon_1 &= 0 \quad \text{(D.32)} \\
F_1 \ y_{C2,1} - \epsilon_2 &= 0 \quad \text{(D.33)} \\
F_1 \ y_{C3,1} - \epsilon_3 &= 0 \quad \text{(D.34)} \\
F_1 \ y_{C4,1} - \epsilon_4 &= 0 \quad \text{(D.35)} \\
F_1 \ y_{C5,1} - \epsilon_5 &= 0 \quad \text{(D.36)}
\end{align*}

And the material balance equations for the rest of the chemical species at the outlet of the combustor are:

\begin{align*}
F_2 \ y_{O2,2} - \left( F_1 \ y_{O2,1} - \frac{7}{2} \epsilon_2 - 5\epsilon_3 - \frac{13}{2} \epsilon_4 - 8\epsilon_5 + \frac{1}{2} \epsilon_6 \right) &= 0 \quad \text{(D.37)} \\
F_2 \ y_{CO2,2} - \left( \epsilon_1 + 2\epsilon_2 + 3\epsilon_3 + 4\epsilon_4 + 5\epsilon_5 - \epsilon_6 \right) &= 0 \quad \text{(D.38)} \\
F_2 \ y_{H2O,2} - \left( 2\epsilon_1 + 3\epsilon_2 + 4\epsilon_3 + 5\epsilon_4 + 6\epsilon_5 - \epsilon_8 - \epsilon_9 \right) &= 0 \quad \text{(D.39)} \\
F_2 \ y_{CO,2} - \epsilon_6 &= 0 \quad \text{(D.40)} \\
F_2 \ y_{N2,2} - \left( F_1 \ y_{N2,1} - \frac{1}{2} \epsilon_7 \right) &= 0 \quad \text{(D.41)} \\
F_2 \ y_{H2,2} - \left( \epsilon_8 + \frac{1}{2} \epsilon_9 - \epsilon_{10} \right) &= 0 \quad \text{(D.42)} \\
F_2 \ y_{OH,2} - \epsilon_9 &= 0 \quad \text{(D.43)} \\
F_2 \ y_{H,2} - 2\epsilon_10 &= 0 \quad \text{(D.44)} \\
F_2 \ y_{O2,2} - 2\epsilon_{11} &= 0 \quad \text{(D.45)} \\
F_2 \ y_{NO,2} - \epsilon_7 &= 0 \quad \text{(D.46)}
\end{align*}

So we have 15 component material balance equations.

\footnote{Note that $y_{i,j}$ is the mole fraction of component $i$ in stream $j$.}
Overall energy balance

Accounts for the heat released and absorbed by each reaction and includes a combustion efficiency,

\[ F_1 h_1 - \left( F_2 h_2 + \eta_c \left[ \Sigma \epsilon_j \Delta H_j(T_0) \right] \right) = 0 \]  
(D.47)

where \( \eta_c \) is the combustion efficiency, \( \epsilon_j \) is the extent of reaction and \( \Delta H_j(T_0) \) is the enthalpy of reaction at the reference temperature. \( j = 1, \ldots, 11 \) involves combustion and equilibrium reactions.

Momentum balance / pressure change

Defines the pressure drop through the combustor in terms of inlet and outlet stream pressures.

\[ P_2 - (P_1 - \Delta P_{cc}) = 0 \]  
(D.48)

Equilibrium relationships

which (i) define the equilibrium constants for the dissociation reactions using:

\[ K_j = \Pi (y_i)^{\nu_{ij}} P^{\nu_j} \]  
(D.49)

and (ii) relate equilibrium constants to temperature:

\[ \ln K_j(T) = -\frac{\Delta G_j}{RT} \]  
(D.50)

We rewrite equation (D.49) as

\[ \ln K_j(T) - \left( \Sigma \nu_{i,j} \ln y_i + \nu_j \ln P \right) = 0 \]  
(D.51)

in order to treat reactants and products symmetrically in terms of nonlinearity in the equation. Thus we have six equations for the equilibrium reactions,

\[ \ln[K_6(T_2)] - \ln(y_{CO2}) - \frac{1}{2} \ln(y_{O2}) + \ln(y_{CO}) - \frac{1}{2} \ln(P_2) = 0 \]  
(D.52)

\[ \ln[K_7(T_2)] - \ln(y_{NO2}) + \frac{1}{2} \ln(y_{N2}) + \frac{1}{2} \ln(y_{O2}) = 0 \]  
(D.53)

\[ \ln[K_8(T_2)] - \ln(y_{H2}) - \frac{1}{2} \ln(y_{O2}) + \ln(y_{H2O}) - \frac{1}{2} \ln(P_2) = 0 \]  
(D.54)

\[ \ln[K_9(T_2)] - \frac{1}{2} \ln(y_{H2}) - \ln(y_{OH}) - \ln(y_{H2O}) - \frac{1}{2} \ln(P_2) = 0 \]  
(D.55)

\[ \ln[K_{10}(T_2)] - 2 \ln(y_{H}) + \ln(y_{H2O}) - \ln(P_2) = 0 \]  
(D.56)

\[ \ln[K_{11}(T_2)] - 2 \ln(y_{O}) + \ln(y_{O2}) - \ln(P_2) = 0 \]  
(D.57)

Note that in equation (D.50) we use:

\[ \Delta G_j = \Delta H_j - T \Delta S_j \]  
(D.58)

\(^3\) In the calculation of equilibrium constants \( \nu_{i,j} \) is the stoichiometric coefficient of the chemical species \( i \) in reaction \( j \), \( \nu_j \) is positive for products and negative for reactants. \( \nu_j \) is the change of moles \( \Sigma \nu_{i,j} \) for the chemical reaction \( j \).
where $\Delta H_j$ and $\Delta S_j$ are calculated by the thermopack from,

$$\Delta H_j = \Delta H_{j,T_0} + \int_{T_0}^{T} \left( \Sigma C_{p_p} - \Sigma C_{p_r} \right)_j dT$$ \hspace{1cm} (D.59)

$$\Delta S_j = \Delta S_{j,T_0} + \int_{T_0}^{T} \frac{\left( \Sigma C_{p_p} - \Sigma C_{p_r} \right)_j}{T} dT$$ \hspace{1cm} (D.60)

there subscripts ‘p’ and ‘r’ refer to products and reactants respectively. $\Delta H_{j,T_0}$, $\Delta S_{j,T_0}$ are respectively the standard heat and entropy of formation for the equilibrium reaction ‘j’ at the reference temperature $T_0$. They are obtained using the stoichiometric coefficients and the enthalpy (or entropy) of formation for products minus that of reactants (Smith and Van Ness, 1987).

Parameters for the calculation of specific heat $C_p$, as explained in Appendix C, as well as standard enthalpy of formation $\Delta H^o_{f,298}$ and standard entropy of formation $\Delta S^o_{f,298}$ are given in Tables D.1 and D.2 (Prothero, 1969), (Smith and Van Ness, 1987). Direct use of such parameters give specific heat and $\Delta S^o_{298}$ in [cal/mole K] and $\Delta H^o_{298}$ in [cal/mole], but were transformed to [kJ/kmol] respectively inside the actual thermopack.

Energy from fuel supplied

This constraint is useful for accounting the energy supplied to the gas turbine $Q_{fuel}$,

$$Q_{fuel} - \Sigma \varepsilon_j \Delta H_j(T_0) = 0$$ \hspace{1cm} (D.61)

for $j = 1, \ldots, 5$ i.e. including just hydrocarbons present in the natural gas considered.

Counting equations, and the outlet stream and performance variables for the combustor reactions section, produces 2 ‘natural’ degrees of freedom which may be taken as: $\Delta P_{cc}$ (the pressure drop through the combustor) and $\eta_c$ (the combustion efficiency).

D.2.3 Expansion section

The expansion section of a gas turbine is modelled as shown in Fig. D.7. This unit receives a hot and pressurised stream from the combustor section so that the expansion process through this turbine produces a total amount of work $W_T$.

The mathematical model for the expansion section considers,

Material balance

The component mole balance equations are given by,

$$F_2 \ y_i = F_1 \ y_i$$ \hspace{1cm} (D.62)

For $N$ components in a stream, we have $N$ component mole balance equations.

Energy balance

$$\eta_M (H_1 - H_2) = W_T$$ \hspace{1cm} (D.63)
Table D.1: Parameters for specific heat of gaseous chemical species and standard enthalpy and entropy of formation.

<table>
<thead>
<tr>
<th>species</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_4$</td>
<td>$0.7918404 \times 10^4$</td>
<td>$-0.1141722 \times 10^2$</td>
<td>$0.6373457 \times 10^2$</td>
<td>$-0.7525691 \times 10^2$</td>
<td>$0.4329269 \times 10^4$</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
<td>$0.2387968408 \times 10^4$</td>
<td>$0.3457751611 \times 10^3$</td>
<td>$0.2497260449 \times 10^4$</td>
<td>$-0.1836373457 \times 10^2$</td>
<td>$0.1038081242 \times 10^2$</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
<td>$0.6800800 \times 10^3$</td>
<td>$0.2871000 \times 10^2$</td>
<td>$0.6234900 \times 10^2$</td>
<td>$-0.1071900 \times 10^3$</td>
<td>$0.6980200 \times 10^2$</td>
</tr>
<tr>
<td>n-C$<em>4$H$</em>{10}$</td>
<td>$-0.3977200 \times 10^2$</td>
<td>$0.4129000 \times 10^3$</td>
<td>$-0.9917400 \times 10^3$</td>
<td>$0.1325000 \times 10^4$</td>
<td>$-0.9267500 \times 10^3$</td>
</tr>
<tr>
<td>n-C$<em>5$H$</em>{12}$</td>
<td>$-0.2857971878 \times 10^3$</td>
<td>$0.1288347906 \times 10^3$</td>
<td>$-0.9084176048 \times 10^2$</td>
<td>$0.4823747357 \times 10^2$</td>
<td>$-0.2197105629 \times 10^2$</td>
</tr>
<tr>
<td>N$_2$</td>
<td>$0.7709928 \times 10^1$</td>
<td>$-0.5503897 \times 10^1$</td>
<td>$0.1312136 \times 10^2$</td>
<td>$-0.1167955 \times 10^2$</td>
<td>$0.5233997 \times 10^1$</td>
</tr>
<tr>
<td>O$_2$</td>
<td>$0.7361141 \times 10^1$</td>
<td>$-0.5369589 \times 10^1$</td>
<td>$0.205179 \times 10^2$</td>
<td>$-0.2586526 \times 10^2$</td>
<td>$0.1594566 \times 10^2$</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>$0.4324933 \times 10^1$</td>
<td>$0.2080895 \times 10^2$</td>
<td>$-0.2294590 \times 10^2$</td>
<td>$0.1684483 \times 10^2$</td>
<td>$-0.7935665 \times 10^1$</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>$0.7988860 \times 10^1$</td>
<td>$-0.1506271 \times 10^1$</td>
<td>$0.6661376 \times 10^1$</td>
<td>$-0.4655970 \times 10^1$</td>
<td>$0.1696464 \times 10^1$</td>
</tr>
<tr>
<td>CO</td>
<td>$0.7812249 \times 10^1$</td>
<td>$-0.6668293 \times 10^1$</td>
<td>$0.1728296 \times 10^2$</td>
<td>$-0.1728709 \times 10^2$</td>
<td>$0.8860125 \times 10^1$</td>
</tr>
<tr>
<td>NO</td>
<td>$0.8462334 \times 10^1$</td>
<td>$-0.1040669 \times 10^2$</td>
<td>$0.2754876 \times 10^2$</td>
<td>$-0.3028119 \times 10^2$</td>
<td>$0.1718511 \times 10^2$</td>
</tr>
<tr>
<td>H$_2$</td>
<td>$0.6183042 \times 10^1$</td>
<td>$0.4710657 \times 10^1$</td>
<td>$-0.1092135 \times 10^2$</td>
<td>$0.1254086 \times 10^2$</td>
<td>$-0.7016263 \times 10^1$</td>
</tr>
<tr>
<td>OH</td>
<td>$0.7615100 \times 10^1$</td>
<td>$-0.1936000 \times 10^1$</td>
<td>$0.8770000$</td>
<td>$0.2615300 \times 10^1$</td>
<td>$-0.2690900 \times 10^1$</td>
</tr>
<tr>
<td>H</td>
<td>$0.4968000 \times 10^1$</td>
<td>$0.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>O</td>
<td>$0.5974134 \times 10^1$</td>
<td>$-0.4241883 \times 10^1$</td>
<td>$0.7931254 \times 10^1$</td>
<td>$-0.7944230 \times 10^1$</td>
<td>$0.4403357 \times 10^1$</td>
</tr>
</tbody>
</table>
Table D.2: Parameters for specific heat of gaseous chemical species and standard enthalpy and entropy of formation (cont.).

<table>
<thead>
<tr>
<th>species</th>
<th>$a_6$</th>
<th>$a_7$</th>
<th>$\Delta H^\circ_{f, 298}$ [cal/mole]</th>
<th>$\Delta S^\circ_{f, 298}$ [cal/mole K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CH_4$</td>
<td>-0.1256732 x10^2</td>
<td>0.1469695 x10^1</td>
<td>-17895.0</td>
<td>44.490</td>
</tr>
<tr>
<td>$C_2H_6$</td>
<td>-0.2320482071 x10^1</td>
<td>0.17140103381</td>
<td>-20033.46080</td>
<td>54.9713</td>
</tr>
<tr>
<td>$C_3H_8$</td>
<td>-0.2110100 x10^2</td>
<td>0.2447600 x10^1</td>
<td>-24891.0</td>
<td>64.355</td>
</tr>
<tr>
<td>n-$C_4H_{10}$</td>
<td>0.3173800 x10^3</td>
<td>-0.4203100 x10^2</td>
<td>-30183.0</td>
<td>74.045</td>
</tr>
<tr>
<td>n-$C_5H_{12}$</td>
<td>0.6792072625 x10^1</td>
<td>-0.9221203575</td>
<td>-35076.48184</td>
<td>83.1739</td>
</tr>
<tr>
<td>$N_2$</td>
<td>-0.1173185 x10^1</td>
<td>0.1038830</td>
<td>0.0</td>
<td>45.77</td>
</tr>
<tr>
<td>$O_2$</td>
<td>-0.4858890 x10^1</td>
<td>0.5861501</td>
<td>0.0</td>
<td>49.004</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>0.2121672 x10^1</td>
<td>-0.2408713</td>
<td>-94054.0</td>
<td>51.072</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>-0.3706212</td>
<td>0.3992444 x10^-1</td>
<td>-57798.0</td>
<td>45.106</td>
</tr>
<tr>
<td>$CO$</td>
<td>-0.2314819 x10^1</td>
<td>0.2447785</td>
<td>-26417.0</td>
<td>47.214</td>
</tr>
<tr>
<td>$NO$</td>
<td>-0.4957260 x10^1</td>
<td>0.5755281</td>
<td>21580.0</td>
<td>50.347</td>
</tr>
<tr>
<td>$H_2$</td>
<td>0.1923395 x10^1</td>
<td>-0.2084091</td>
<td>0.0</td>
<td>31.208</td>
</tr>
<tr>
<td>$OH$</td>
<td>0.9778900</td>
<td>-0.1269500</td>
<td>9432.0</td>
<td>43.88</td>
</tr>
<tr>
<td>$H$</td>
<td>0.0</td>
<td>0.0</td>
<td>52100.0</td>
<td>27.392</td>
</tr>
<tr>
<td>$O$</td>
<td>-0.1271341 x10^1</td>
<td>0.1491408</td>
<td>59559.0</td>
<td>38.468</td>
</tr>
</tbody>
</table>

Figure D.7: Model for the expansion section in a gas turbine.
where $\eta_M$ is the mechanical efficiency.

**Momentum balance / pressure change**

In the same way as in the compressor section, an equation to relate inlet and outlet pressure is required,

$$P_2 \, r_{ep} = P_1$$  \hspace{1cm} (D.64)

where $r_{ep}$ is the expander pressure ratio.

**Performance equations**

One is for the isentropic efficiency,

$$h_1 - h_2 = \eta_{iso} \, (h_1 - h_{iso})$$  \hspace{1cm} (D.65)

And two more equations for the isentropic outlet conditions,

$$h_{iso} = h_{stream}(P_2, T_{iso}, y_i)$$  \hspace{1cm} (D.66)

$$s_1 = s_{stream}(P_2, T_{iso}, y_i)$$  \hspace{1cm} (D.67)

**Number of Degrees of Freedom**

The expansion section should be responsible for the independent variables $F_2, P_2, h_2$ and $(N-1)$ of the mole fractions $y_i$ for the material stream OUT. And also for the unit variables: $W_T, r_{ep}, \eta_M, \eta_{iso}, h_{iso}$ and $T_{iso}$. So, the number of degrees of freedom is:

$$[(3 + (N - 1) + 6)] - (N + 1 + 1 + 3) = 3$$

Thus, the ‘natural’ degrees of freedom for the expansion section of a gas turbine are: $r_{ep}, \eta_M$ and $\eta_{iso}$.

**D.3 Heat recovery (HR) exchanger**

This model considers waste heat recovery coils used to recover heat from a gas turbine exhaust.

**Material streams**

As can be observed from Fig. D.8 a heat recovery exchanger has 2 inlet and 2 outlet material streams. The local stream names are: HOT IN, HOT OUT, COLD IN and COLD OUT. And the local stream numbers: 1, 2, 3, 4.

**Material, energy and momentum balances**

- **Hot side:**
  
  There are $N$ mole balance equations like:

  $$F_2 \, y_{i,2} = F_1 \, y_{i,1}$$  \hspace{1cm} (D.68)
While the energy balance is:

$$H_2 = H_1 - \frac{Q}{\eta_{HX}}$$  \hspace{1cm} (D.69)

where $Q$ is the heat load and $\eta_{HX}$ is the waste heat exchange efficiency (Ganapathy, 1996) which is equal to one minus the heat loss fraction (0.01 is recommended).

Now, for convenience the energy balance is written as,

$$\eta_{HX} (H_2 - H_1) = -Q$$  \hspace{1cm} (D.70)

And the momentum balance,

$$P_2 = P_1 - \Delta P_{hs}$$  \hspace{1cm} (D.71)

where subscript ‘hs’ refers to hot side.

- **Cold side:**

  This is water or steam, so the material balance equation is:

  $$F_4 = F_3$$  \hspace{1cm} (D.72)

\footnote{Note that a separate water/steam thermodynamic package has been developed having different stream definition to the “hot side” in this heat exchange section.}
The energy balance equation is:
\[ H_4 = H_3 + Q \] (D.73)

The momentum balance is given by,
\[ P_4 = P_3 - \Delta P_{cs} \] (D.74)

where subscript 'cs' refers to cold side stream.

**Performance equations**

**Heat transfer equation**, 
\[ Q = (UA) LMTD Ft \] (D.75)

where, 'UA' is a single variable considering the product of the overall heat transfer coefficient 'U' and the heat transfer area 'A'. And:  
\[ LMTD = \frac{(T_1 - T_4) - (T_2 - T_3)}{\ln \left( \frac{T_1 - T_4}{T_2 - T_3} \right)} \]

Also in equation (D.75) we have included the form factor \( Ft \) even though in the design practice of HRSG some authors e.g. (Ganapathy, 1996), (Ganapathy, 1991) do not account for \( Ft \) in the heat transfer calculation.

It may be desirable in equation (D.75) to have the approach temperatures \( DT \) (e.g. \( T_1 - T_4 \)) as explicit variables because they may be subject to heat recovery optimisation. Thus the two additional modelling equations are,
\[ DT_h = (T_1 - T_4) \] (D.76)
\[ DT_c = (T_2 - T_3) \] (D.77)

So equation (D.75) can be expressed as,
\[ Q = (UA) \left[ \frac{(DT_h) - (DT_c)}{\ln \left( \frac{DT_h}{DT_c} \right)} \right] Ft \] (D.78)

The unpleasant features of the last equation in equation-based modelling like \( (T_1 - T_4) = (T_2 - T_3) \), are solved by using the "grey box formulation" (Morton, 1996),
\[ LMTD = (T_2 - T_3) f(\alpha) = DT_c f(\alpha) \]

where,
\[ \alpha = \frac{(T_1 - T_4)}{(T_2 - T_3)} = \frac{(DT_h)}{(DT_c)} \]
\[ f(\alpha) = \frac{\alpha - 1}{\ln(\alpha)} \]

except when \(|\alpha - 1| < 0.01\) and in this case,
\[ f(\alpha) = 1 + \frac{\alpha - 1}{2} - \frac{(\alpha - 1)^2}{12} \]

\(^5\) The Logarithmic Mean Temperature Difference (LMTD) for a heat recovery section is calculated in the same way as for simple countercurrent heat exchange (Ganapathy, 1996).
Number of Degrees of Freedom

The heat exchange section should be responsible for the independent variables $F_2$, $P_2$, $h_2$ and $(N - 1)$ of mole fractions $y_i$ for the material hot stream OUT. Also for the independent variables $F_4$, $P_4$, $h_4$ of the material cold stream OUT and for the unit variables: $Q$, $\eta_{HX}$, $\Delta P_{hs}$, $\Delta P_{cs}$, $UA$, $DT_h$, $DT_c$ and $F_t$. So, the number of degrees of freedom is:

$$[(3 + (N - 1) + 3 + 8) - (N + 2 + 3 + 1 + 2) = 5$$

Thus, the ‘natural’ degrees of freedom for a heat recovery exchanger are: $\eta_{HX}$, $\Delta P_{hs}$, $\Delta P_{cs}$, $F_t$, $UA$.

It is important to mention that in this model the heat transfer equation (D.78) considers the product ‘$UA$’ as a single variable. In this way some problems including the profit optimisation for a real cogeneration plant (Chapter 7, Section 7.6) were solved. When the heat transfer area ‘$A$’ was needed for economic optimisation and synthesis problems (see Chapters 7-8), the constraint having the two variables explicitly,

$$UA = U \times A$$

was added.

D.4 Steam drum

A heat recovery steam generator (HRSG) can have several steam pressure levels. A steam drum is required for each pressure level, to separate water from steam which is sent for superheating in the waste heat recovery boiler. The steam drum also helps to stabilise the operation as it connects the water/steam streams between the different heat exchange sections into the HRSG.

Material streams

From Fig. D.9 note that the steam drum section has 2 inlet and 2 outlet material streams. Local stream names are: WATER IN, SATURATED WATER OUT, SATURATED STEAM IN and SATURATED STEAM OUT. While local stream numbers are: 1, 2, 3, 4.

Material balance

$$F_1 + F_3 = F_2 + F_4 \quad \text{(D.79)}$$

Energy balance

$$H_1 + H_3 = H_2 + H_4 \quad \text{(D.80)}$$

Momentum balance equations

$$P_2 = P_1 \quad \text{(D.81)}$$
$$P_3 = P_2 \quad \text{(D.82)}$$
$$P_4 = P_3 \quad \text{(D.83)}$$

Performance equations
One performance equation is for accounting the "steam drum approach point", $\Delta T_{Drum}$ as proposed in (Ganapathy, 1991). This is defined as the difference between the saturation temperature $T_s$ of the water stream going to the steam drum and its actual temperature or:

$$\Delta T_{Drum} = T_{s,1} - T_1$$

(D.84)

Since the steam drum sends saturated water to the evaporator and then sends dry saturated steam to the superheating section (stream 4 in Fig. D.9) ensuring phase separation from the steam drum, then the following equations should be satisfied,

The steam drum should send saturated liquid (see Fig. D.9 and Fig. D.10) so we have:

$$q_2 = 1.0$$

(D.85)

In addition, the steam drum should be able to send dry saturated steam,

$$q_4 = 0.0$$

(D.86)

**Number of Degrees of Freedom**

The steam drum section should be responsible for the independent variables $F_2$, $P_2$, $h_2$ and $F_4$, $P_4$, $h_4$ of the material streams OUT and the defined local variable: $\Delta T_{Drum}$. Thus, the number of degrees of freedom is,

$$(3 + 3 + 1) - (1 + 1 + 3 + 1 + 1 + 1) = -1$$

This 'negative' degree of freedom (or degree of constraint) is associated with the fact that the two inlet streams are forced to have the same pressure.

---

6 For stream 2 in Fig. D.9 the stream quality ($q$) is obtained from,

$$q_2 = \frac{h_{g,2} - h_2}{h_{g,2} - h_{f,2}}$$
D.5 Heat recovery steam generator (HRSG)

The exhaust gas of a gas turbine is hot enough to generate steam at different pressure levels, for use as process steam, for deaeration or in steam turbines for additional power generation. A simple HRSG is represented in Fig. D.10 where subcooled water is passed through a section of heat exchange then gets a temperature close to its saturation point (but slightly below to avoid vaporisation within this section). This part of the HRSG is called the economiser. From the economiser water goes to the steam drum where saturated liquid water is sent to the evaporation section to obtain saturated steam which is sent back to the steam drum where is then distributed to the superheating section. The HRSG produces steam coming from the superheating section.

The fundamental model of a HRSG consists of a series of heat recovery exchangers (Section D.3) and a steam drum (Section D.4) models connected appropriately. For a given HRSG model the Number of Degrees of Freedom is obtained by the difference between variables and equations for all streams and unit operations involved (see e.g. Chapter 6, Section 6.4.3 on page 121).

D.6 Deaerator

An important unit operation in utility systems is the deaerator which eliminates dissolved oxygen in condensate water. In a steam system a quantity of raw water makeup is added in order to compensate any steam or water losses by purge for steady state operation. Makeup water has a small quantity of dissolved gases (e.g. oxygen and carbon dioxide) and condensate absorbs the dissolved gases after makeup water is incorporated to the steam system. These dissolved gases produce corrosion in the HRSG heat transfer tubing. Small amounts of oxygen
in the steam system cause severe chemical attack at the operating temperatures within the system. For this reason, oxygen should be removed from HRSG feed water (Ketten, 1986).

In many steam plants deaeration is carried out in two stages: mechanical followed by chemical deaeration. However, our approach is to model only mechanical deaeration since it is directly related to steam consumption which has the major effect in our optimisation problems.

In mechanical deaeration oxygen is removed practically in full. Removal is based on two physical laws: i) Charles' Law which predicts that the solubility of gases in liquids decreases with temperature and ii) Henry's Law which predicts that the concentration of a dissolved gas in solution is proportional to the partial pressure of the gas in the free space above the liquid.

Oxygen in the condensate of a steam system can be removed by heating and by reducing the partial pressure of oxygen in the surroundings of the liquid. The easiest way to deaerate water is to bubble or spray the condensate in counterflow with steam (the scrubbing medium) and to vent the oxygen. The oxygen concentration in the liquid decreases proportionally to the reduction in its partial pressure.

The model for this equipment involves fundamental balances, equations for the concentration in ppm (parts per million) of dissolved oxygen to and from the deaerator and a rigorous representation of dissolved oxygen concentration as a function of pressure and temperature.

A schematic diagram for the deaerator is shown in Fig. D.11.

**Material streams**

From Fig. D.11 note that the deaerator has 2 inlet and 2 outlet material streams. Local stream names: WATER IN, (low pressure) LP STEAM IN, WATER OUT and VENT OUT. Local stream numbers: 1, 2, 3, 4.
Total Material balance

\[ F_3 + F_4 = F_1 + F_2 \]  (D.87)

Oxygen Material balance

\[ F_3 \left( x_{W_{O_{2,3}}} \right) + F_4 \left( x_{W_{O_{2,4}}} \right) = F_1 \left( x_{W_{O_{2,1}}} \right) + F_2 \left( x_{W_{O_{2,2}}} \right) \]

Where \( x_{W_{O_{2,1}}} \), \( x_{W_{O_{2,2}}} \), \( x_{W_{O_{2,3}}} \) and \( x_{W_{O_{2,4}}} \) are the mass ratio of dissolved oxygen in streams 1, 2, 3 and 4 respectively (for simplicity, calculated as mass fraction).

Note that the concentration of \( O_2 \) in streams 2 (LP steam) and 3 (deaerated water) is the same since LP steam is produced from the deaerated water from this equipment. Thus, the oxygen material balance can be simplified as,

\[ F_3 \left( x_{W_{O_{2,3}}} \right) + F_4 \left( x_{W_{O_{2,4}}} \right) = F_1 \left( x_{W_{O_{2,1}}} \right) + F_2 \left( x_{W_{O_{2,1}}} \right) \]  (D.88)

Energy balance

\[ H_3 + H_4 = H_1 + H_2 \]  (D.89)

Momentum balance equations

\[ P_2 = P_1 \]  (D.90)
\[ P_3 = P_2 \]  (D.91)
\[ P_4 = P_3 \]  (D.92)

Performance equations

There is one performance equation for the quantity of dissolved oxygen in liquid water (Fogg and Gerrard, 1991), which in mole fraction units is,

\[ x_{O_2} = \exp \left( -139.485 + \frac{6889.6}{T} + 18.554 \ln (T) \right) \]

Such an expression is valid for a partial pressure of oxygen of 1.013 bar and a temperature range \( (273K \leq T \leq 617K) \) thus covering any practicable deaerator operating temperatures. That expression has a standard deviation of 2.0% (Fogg and Gerrard, 1991).

The streams involved in a deaerator obviously have an oxygen partial pressures smaller than 1.013 bar (since in utility systems they are not in contact with a pure-oxygen atmosphere). Thus, without loss of applicability of our equation for the dissolved oxygen in water, we can linearly interpolate to smaller (less than 1.013 bar) partial pressures of oxygen (Goodall, 1981) so,

\[ x_{O_2} = \left[ \exp \left( -139.485 + \frac{6889.6}{T} + 18.554 \ln (T) \right) \right] y_{O_2} P \]

In the last equation \( y_{O_2} \) is the oxygen mole fraction in the vapour phase. The total pressure \( P \), should be consistent in units with the pressure at which the correlation for the dissolved oxygen in water was obtained (Fogg and Gerrard, 1991).
So that our performance equation is,
\[ x_{O_{2,3}} = \left( \exp \left( -139.485 + \frac{6889.6}{T_3} + 18.554 \ln (T_3) \right) \right) y_{O_{2,4}} P_4 \]  \hspace{1cm} (D.93)

In equation (D.88) \( x_{W_{O_{2,3}}} \) and \( x_{W_{O_{2,4}}} \) are the mass fractions of dissolved oxygen in streams 3 and 4 respectively. We need two extra equations to relate mole fraction variables from equation (D.93) with their corresponding mass fraction values,
\[ x_{W_{O_{2,3}}} = x_{O_{2,3}} \left( \frac{32.0}{18.0} \right) \]  \hspace{1cm} (D.94)
\[ x_{W_{O_{2,4}}} = y_{O_{2,4}} \left( \frac{32.0}{18.0} \right) \]  \hspace{1cm} (D.95)

Finally, since we are interested in knowing the ppm (parts per million) of dissolved oxygen in the water streams involved, two additional modelling equations are needed,
\[ ppm_{O_{2,1}} = x_{W_{O_{2,1}}} \left( 1.0 \times 10^6 \right) \]  \hspace{1cm} (D.96)
\[ ppm_{O_{2,3}} = x_{W_{O_{2,3}}} \left( 1.0 \times 10^6 \right) \]  \hspace{1cm} (D.97)

**Number of Degrees of Freedom**

The deaerator unit should be responsible for the independent variables \( F_3, P_3, h_3 \) and \( F_4, P_4, h_4 \) of the material streams OUT as well as for the introduced variables: \( x_{W_{O_{2,1}}}, x_{W_{O_{2,3}}}, x_{W_{O_{2,4}}}, y_{O_{2,4}}, \) and \( ppm_{O_{2,1}}, ppm_{O_{2,3}} \). So the number of degrees of freedom is,
\[ (3 + 3 + 3 + 2 + 2) - (1 + 1 + 1 + 1 + 2 + 2) = 13 - 11 = 2 \]

Thus, the 'natural' degrees of freedom for a deaerator are \( ppm_{O_{2,1}} \) (the quantity of dissolved oxygen in the water to be deaerated) and \( ppm_{O_{2,3}} \) (the desired quantity of dissolved oxygen in the deaerated water).

In our CHP systems we specified \( ppm_{O_{2,1}} = 7 \) and \( ppm_{O_{2,3}} = 0.007 \) (Goodall, 1981).

**D.7 Air-cooled condenser**

**Material streams**

From Fig. D.12 note that an air-cooled steam condenser has 2 inlet and 2 outlet material streams. Local stream names: STEAM IN, CONDENSATE OUT, AIR IN, AIR OUT. Local stream numbers: 1, 2, 3, 4.

**Material, energy and momentum balances**

- Hot side (steam):
\[ F_2 = F_1 \]  \hspace{1cm} (D.98)
\[ H_2 = H_1 - Q \]  \hspace{1cm} (D.99)
\[ P_2 = P_1 - \Delta P_{hs} \]  \hspace{1cm} (D.100)
Figure D.12: Model for an air-cooled steam condenser.

- Cold side (air single component stream):
  \[
  F_4 = F_3 \quad (D.101)
  \]
  \[
  H_4 = H_3 + Q \quad (D.102)
  \]
  \[
  P_4 = P_3 - \Delta P_{cs} \quad (D.103)
  \]

**Performance equations**

Heat transfer equation,

\[
Q = (UA) \left[ \frac{(DT_h - DT_c)}{\ln \left( \frac{DT_h}{DT_c} \right)} \right] F_t
\]

where,

\[
DT_h = (T_1 - T_4) \quad (D.105)
\]
\[
DT_c = (T_2 - T_3) \quad (D.106)
\]

We use the same continuous approximation for the LMTD as explained in Section D.3.

The LMTD correction factor ‘\(F_t\)’ for cross flow heat exchange can be obtained from (Roetzel and Nicole, 1975),

\[
F_t = 1 - \sum_{i=1}^{4} \sum_{k=1}^{4} a_{i,k} \left( 1 - \phi_3 \right)^k \sin \left[ 2i \arctan \left( \frac{\phi_1}{\phi_2} \right) \right]
\]

\[(D.107)\]
where (for the stream numbers as given in Fig. D.12),

\[
\phi_1 = \frac{T_1 - T_2}{T_1 - T_3} \\
\phi_2 = \frac{T_4 - T_2}{T_1 - T_3} \\
\phi_3 = \frac{\phi_1 - \phi_2}{\ln \left( \frac{1 - \phi_2}{1 - \phi_1} \right)}
\]

And the values of \( a_{i,k} \) are specific for a heat exchanger configuration. We use parameters for a four-row two-passes tube-side condenser shown in Table D.3.

<table>
<thead>
<tr>
<th>( i = 1 )</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k = 1 )</td>
<td>-6.06 \times 10^{-1}</td>
<td>2.31 \times 10^{-2}</td>
<td>2.94 \times 10^{-1}</td>
</tr>
<tr>
<td>2</td>
<td>4.34 \times 10^0</td>
<td>5.90 \times 10^{-3}</td>
<td>-1.99 \times 10^0</td>
</tr>
<tr>
<td>3</td>
<td>-9.72 \times 10^0</td>
<td>-2.48 \times 10^{-1}</td>
<td>4.32 \times 10^0</td>
</tr>
<tr>
<td>4</td>
<td>7.54 \times 10^0</td>
<td>2.87 \times 10^{-1}</td>
<td>-3.0 \times 10^0</td>
</tr>
</tbody>
</table>

In order to have realistic models some design considerations should be applied. One is the concept of the Terminal Temperature Difference, \( (TTD) \) which is the difference between the condensing turbine exhaust and the condensate outlet temperatures (Conradie and Kröger, 1996).  

In real plants the \( TTD \) is caused mainly by frictional effects (Conradie and Kröger, 1996) and could be expressed as,

\[
TTD = T_{s_1} - T_2
\]  

where \( T_{s_1} \) is the saturation temperature of the steam entering the air cooler.

A simplified form for obtaining the fan power \( W_f \) for this equipment is (Ulrich, 1984),

\[
W_f = \frac{F_3 \Delta P_{cs} \bar{v}}{\eta_F}
\]

where \( \eta_F \) is the fan-motor mechanical efficiency and \( \bar{v} \) is the average air specific volume, \([m^3/kg] \). obtained from,

\[
\bar{v} = 0.5 \left[ v(T_3, P_3) + v(T_4, P_4) \right]
\]

The last equation implied the necessity to include air specific volume (one variable and one constraint) into our original air single component stream model (see Chapter 3, Section 3.1.2).

---

7 A value of \( TTD \) from 2 to 4 °C is suggested.
Number of Degrees of Freedom

An air-cooled steam condenser should be responsible for the independent variables $F_2, P_2, h_2$ and $F_4, P_4, h_4$ of the material streams OUT as well as the introduced variables: $Q, (UA), F_t, DT_h, DT_c, TTD, W_f, \Delta P_{hs}, \Delta P_{cs}, 6, \eta_F$. Thus the number of degrees of freedom is,

$$(3 + 3 + 11) - (3 + 3 + 7) = 4$$

The 'natural' degrees of freedom for an air-cooled steam condenser are: $\Delta P_{hs}, \Delta P_{cs}, (UA)$ and $\eta_F$.

Again in this model the heat transfer equation (D.104) considers the product $(UA)$ as a single variable. When the heat transfer area $A$ was needed for economic optimisation and synthesis problems (see e.g. Chapter 7, Section 7.5.1 and Chapter 8), the constraint having the two variables explicitly,

$$UA = U \times A$$

was added.

D.8 Pump

From Fig. D.13 note that a pump has 1 inlet and 1 outlet material streams. This is a simple model which uses similar equations as the compressor model, but this involves liquid streams.

![Figure D.13: Model for a pump.](image)

Material balance

$$F_2 = F_1 \quad \text{(D.111)}$$

Energy balance

$$H_2 = H_1 + \eta_p W \quad \text{(D.112)}$$

* a recommended value for the air pressure drop is $\Delta P_{cs} = 1.2 \times 10^{-4} \text{ MPa}$ (Ulrich, 1984).
where $\eta_p$ is the pump efficiency. This depends really on pump size, and for centrifugal pump (with capacity of 0.25 to $1000 \: m^3/hr$ i.e. from $0.0694$ to $277.778 \: kg/s$) varies from 50 to 90% approximately. $W$ is the power required for pumping.

**Momentum balance equation**

\[ P_2 = P_1 + \Delta P \]  \hspace{1cm} (D.113)

**Performance equations**

\[
\begin{align*}
\delta_{i\theta} - \delta_1 &= \eta_{i\theta}(\delta_2 - \delta_1) \\
\delta_{i\theta} &= \phi_{i\theta} \: \delta_{i\theta}(T_{i\theta}, P_2) + (1 - \phi_{i\theta}) \: \delta_{i\theta}(T_{i\theta}, P_2) \\
\delta_1 &= \phi_{i\theta} \: \delta_{i\theta}(T_{i\theta}, P_2) + (1 - \phi_{i\theta}) \: \delta_{i\theta}(T_{i\theta}, P_2) \\
\phi_{i\theta} + a_{i\theta} \: q_{i\theta} &= \delta_{i\theta} \\
q_{i\theta} &= \frac{(\delta_{i\theta} - \delta_{i\theta})}{(\delta_{i\theta} + \delta_{i\theta})}
\end{align*}
\]  \hspace{1cm} (D.114)-(D.118)

**Number of Degrees of Freedom**

Independent variables for outlet stream and unit local variables minus model equations produce 3 ‘natural’ degrees of freedom: $\Delta P$, $\eta_p$ and $\eta_{i\theta}$.

**D.9 Water/water heat exchanger**

This is a similar model to the heat recovery exchanger (Section D.3), but of course here we have water streams in both the shell and the tube sides of the exchanger. The model for water/water heat exchanger was then easily constructed.

**D.10 Mixer/splitter (multi-component streams)**

The superstructure model required a gas turbine exhaust mixer/splitter with the capability of having any number of IN/OUT streams.

A multicomponent stream mixer/splitter was modelled according to Fig. D.14.

**Material streams**

This mixer/splitter has $N._{IN}$ inlet and $N._{OUT}$ outlet material streams.

Here the local stream names are: $IN._1$ to $N._{IN}$ and $OUT._1$ to $N._{OUT}$.

While the local stream numbers are: 1 to $N._{IN}$, $N._{IN} + 1$ to $N._{IN} + N._{OUT}$.

**Material balances**
APPENDIX D. EQUATION ORIENTED UNIT OPERATIONS MODELS

Figure D.14: Model for a mixer/splitter.

For a total number of components \( N_{TC} \) going to the mixer/splitter through the different \( N_{IN} \) streams we have \( N_{TC} \) component mole balance equations given by,

\[
\sum_{j=1}^{N_{OUT}} F_{N_{IN}+j} \cdot y_{i,N_{IN}+j} = \sum_{j=1}^{N_{IN}} F_{j} \cdot y_{i,j} \quad (D.119)
\]

where \( i = 1, ..., N_{TC} \)

Energy balance

\[
\sum_{j=1}^{N_{OUT}} H_{N_{IN}+j} = \sum_{j=1}^{N_{IN}} H_{j} \quad (D.120)
\]

Momentum balances

There are \( N_{IN} + N_{OUT} - 1 \) momentum balance equations.

All pressures are equal around the mixer/splitter,

\[
P_{j+1} = P_{j} \quad (D.121)
\]

where \( j = 1, ..., N_{IN} + N_{OUT} - 1 \)

Equal outlet properties

Equations for the equal enthalpy and equal outlet composition of the outlet streams are needed. This is because the intensive properties needed to define a multicomponent stream in single phase, according to the phase rule are,

\[
f = N_C - P + 2 = N_C - 1 + 2
\]

i.e. the mole fraction of all except one component, \( P \) and \( h \).

Therefore we have:
• Equal outlet enthalpy equations
  \( N_{OUT} - 1 \) equations of the form,
  \[ h_{j+1} = h_j \]  \hspace{1cm} (D.122)
  For \((j = N.IN + 1, \ldots, N.IN + N.OUT - 1)\)

• Equal outlet composition equations
  The number of equal outlet mole fraction equations is \((N.TC - 1) (N.OUT - 1)\) each
  being of the form,
  \[ y_{i, j+1} = y_{i, j} \]  \hspace{1cm} (D.123)
  where \((i = 1, \ldots, N.TC - 1\) and \(j = N.IN + 1, \ldots, N.IN + N.OUT - 1)\)

**Number of Degrees of Freedom**

This mixer/splitter should be responsible for the independent variables: \(F, P, h\) and \((N.TC - 1)\)
  of the component mole fraction \(y_i\) for the outlet streams \(N.OUT\). Therefore, the number of
degrees of freedom is,

\[
\begin{align*}
3 (N.OUT) + N.OUT (N.TC - 1) & - \\
[N.TC + 1 + (N.IN + N.OUT - 1) + (N.OUT - 1) + (N.TC - 1) (N.OUT - 1)] & = \\
2 N.OUT + N.OUT N.TC - (N.IN + N.OUT + N.OUT N.TC) & = N.OUT - N.IN
\end{align*}
\]

In other words, this unit should be responsible for the degrees of freedom of the outlet streams
minus the degrees of freedom of the inlet streams, or:

- \(N.OUT - 1\) outlet stream flows (for all but one OUT stream)
- \(N.IN - 1\) stream pressures (for all but one IN stream)
- \(N.OUT - N.IN\)

**D.11 Mixer/splitter (single component streams)**

This model is represented with the same schematic diagram presented for the mixer-splitter for
multicomponent streams (Section D.10, Fig. D.14).

**Material balance**

\[
\begin{align*}
\sum_{j=1}^{N.OUT} F_{N.IN+j} & = \sum_{j=1}^{N.IN} F_j \\
N.OUT & = N.IN
\end{align*}
\]  \hspace{1cm} (D.124)

**Energy balance**

\[
\begin{align*}
\sum_{j=1}^{N.OUT} H_{N.IN+j} & = \sum_{j=1}^{N.IN} H_j \\
N.OUT & = N.IN
\end{align*}
\]  \hspace{1cm} (D.125)
Momentum balances

\[ P_{j+1} = P_j \]  
(D.126)

where \((j = 1, ..., N.IN + N.OUT - 1)\)

Equal outlet properties

For a single component stream we have only equal outlet enthalpy equations. \(N.OUT - 1\) equations of the form,

\[ h_{j+1} = h_j \]  
(D.127)

For \((j = N.IN + 1, \ldots, N.IN + N.OUT - 1)\)

Number of Degrees of Freedom

This mixer/splitter should be responsible for the independent variables: \(F, P, h\) of the outlet streams \(N.OUT\). The corresponding the number of degrees of freedom is,

\[ N.OUT - N.IN \]

D.12 Compressor

This unit illustrated in Fig. D.15 considers compression of air in its single component model.

Material balance

\[ F_2 = F_1 \]  
(D.128)

Figure D.15: Model for a compressor.
Energy balance

\[ H_2 = H_1 + \eta_M W \]  \hspace{1cm} (D.129)

where \( \eta_M \) is the mechanical efficiency.

Momentum balance equation

\[ P_2 = P_1 + \Delta P \]  \hspace{1cm} (D.130)

Performance equations

\[ h_{iso} - h_1 = \eta_{iso} (h_2 - h_1) \]  \hspace{1cm} (D.131)
\[ h_{iso} = h_a (T_{iso}, P_2) \]  \hspace{1cm} (D.132)
\[ s_1 = s_a (T_{iso}, P_2) \]  \hspace{1cm} (D.133)

Number of Degrees of Freedom

The number of independent variables for stream OUT and unit local variables minus model equations produce 3 'natural' degrees of freedom: \( \Delta P \), \( \eta_M \) and \( \eta_{iso} \).

D.13 Heater/cooler

This is a simple model represented in Fig. D.16 where no heat transfer equation is included, but the unit heat load is determined under the energy balance exclusively. This is a useful model in applications where no details are given for the heat transfer units e.g. steam load exported to an external site from a cogeneration system.

Material balance

\[ F_2 = F_1 \]  \hspace{1cm} (D.134)

Energy balance

\[ H_2 = H_1 + Q \]  \hspace{1cm} (D.135)

Figure D.16: Model for a heater/cooler.
Momentum balance

\[ P_2 = P_1 - \Delta P \]  
(D.136)

where \( \Delta P \) is the pressure drop across the heater/cooler.

Number of Degrees of Freedom

Obtained as 2. The 'natural' degrees of freedom for this unit are: \( \Delta P \) and \( Q \)

D.14 Valve

A valve is illustrated in Fig. D.17.

Material balance

\[ F_2 = F_1 \]  
(D.137)

Energy balance

\[ H_2 = H_1 \]  
(D.138)

Momentum balance

\[ P_2 = P_1 - \Delta P \]  
(D.139)

Number of Degrees of Freedom

A valve should be responsible for the independent variables \( F_2, P_2 \) and \( h_2 \) of the material stream OUT as well as the unit variable which has been introduced \( \Delta P \). Thus, the number of degrees of freedom is:

\[ (3 + 1) - (1 + 1 + 1) = 1 \]

The 'natural' degree of freedom for a valve is: \( \Delta P \).

Figure D.17: Model for a valve.
## D.15 Specifications for heat transfer coefficients

Overall heat transfer coefficients $U$ are presented in Table D.4.

Note that superscripts (a) and (b) in Table D.4 are described as follows: (a) was obtained as the average between the upper and lower bounds; while (b) was calculated from the simulation of a real cogeneration plant (Gator-Power, 1994).

Table D.4: Overall heat transfer coefficients, $U$ [kW/ m$^2$ °C].

<table>
<thead>
<tr>
<th>Heat exchanger</th>
<th>$U$ (general / applied here)</th>
<th>citation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water/water</td>
<td>1.14 - 1.42 / 1.28 (a)</td>
<td>(Ulrich, 1984)</td>
</tr>
<tr>
<td>Gas/water</td>
<td>0.0113568 - 0.28392 / 0.03199221 (b)</td>
<td>(Peters and Timmerhaus, 1991)</td>
</tr>
<tr>
<td>Steam/gases</td>
<td>0.028392 - 0.28392 / 0.029366 (b)</td>
<td>(Peters and Timmerhaus, 1991)</td>
</tr>
<tr>
<td>Air-cooled steam condenser</td>
<td>0.79 - 0.85 / 0.82 (a)</td>
<td>(Ulrich, 1984)</td>
</tr>
<tr>
<td>Steam generator</td>
<td>0.0406924 / 0.0369407 (b)</td>
<td>(Ganapathy, 1991)</td>
</tr>
</tbody>
</table>
Appendix E

Economic data

This appendix shows data for capital cost of equipment and operating costs for the utilities present in combined heat and power (CHP) systems. In addition, here are shown equipment installation factors, which are needed for the calculation of the installed equipment costs as explained in Chapter 3, Section 3.4.2. For the optimisation and synthesis problems operating and capital cost were expressed in 1997 costs using the corresponding "Chemical Engineering Plant Cost Index", CE index (Ulrich, 1992).

In order to get annualised equipment capital cost a repayment multiplier \( r = 0.15 \), as in (Papoulias and Grossmann, 1983a), was used in the general economic objective function described in Chapter 3, Section 3.4.2. This value for \( r \) was used for the optimisation and synthesis problems and corresponds to 20 years project life and an annual interest of 13.89%. Annualised operating costs assumed operation for 8,400 hour/year as in (Colmenares and Seider, 1989).

Operating and capital costs are for the corresponding year for which data were available in the open literature. If the year for a given cost data was not explicitly mentioned in the relevant reference, then we assume that the cost was for the year of publication.

E.1 Operating costs

The operating costs considered are shown in Table E.1. This table has the cost in U.S. Dollars for utilities with the corresponding year for which data were available along with the relevant bibliographic citation.

E.2 Capital costs

Table E.2 shows the capital costs for equipment in CHP systems. For every type of unit the cost function, the year for which data were available and the bibliographic citation are given. Some of the cost functions were available in the open literature for purchase cost of equipment.
Table E.1: Operating Costs.

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
<th>Year</th>
<th>Citation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity ($/kWh)</td>
<td>$C_{el} = 0.07$</td>
<td>1990</td>
<td>(Ulrich, 1992)</td>
</tr>
<tr>
<td>Natural gas ($/kWh)</td>
<td>$C_{gas} = 0.018$</td>
<td>1990</td>
<td>(Ulrich, 1992)</td>
</tr>
<tr>
<td>Process steam ($/kg)</td>
<td>$C_{st} = \left[ \frac{2.7 \times 10^{-6}}{P^{0.8}} \right] CE \text{ index} + 0.0034 \left[ P^{0.005} \right] C_{gas,GJ}$</td>
<td>1990</td>
<td>(Ulrich, 1992)</td>
</tr>
<tr>
<td>Demineralized (boiler feed) make-up water ($/m^3$)</td>
<td>$C_{H2O} = \left[ 0.007 + \frac{1.3 \times 10^{-6}}{q} \right] CE \text{ index} + 0.0022 C_{gas,GJ}$</td>
<td>1990</td>
<td>(Ulrich, 1992)</td>
</tr>
<tr>
<td></td>
<td>$C_{gas,GJ} = $ 5.0/GJ; \ 0.001 &lt; q &lt; 1.0 \text{ m}^3/s$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Operation and maintenance ($/kWh$)</td>
<td>$C_{om} = $0.02$ (for electricity produced)</td>
<td>1995</td>
<td>(Roy-Aikins, 1995)</td>
</tr>
</tbody>
</table>
Table E.2: Capital costs.

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
<th>Year</th>
<th>Citation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shell and tube HX (k$)</td>
<td>$C = 30.8 + 0.75A^{0.81}$</td>
<td>1989</td>
<td>(Ahmad et al., 1990)</td>
</tr>
<tr>
<td>Steam turbine (k$ /yr)</td>
<td>$482.993 + 0.2627W - 0.7024 \times 10^{-6} W^2$</td>
<td>1992</td>
<td>(Maia et al., 1995)</td>
</tr>
<tr>
<td>Air-cooled HX (k$)</td>
<td>$3.7136A^{0.4015}$</td>
<td>1982</td>
<td>(Ulrich, 1984)</td>
</tr>
<tr>
<td>Deaerator (k$ /yr)</td>
<td>$2.0 F^{0.62}$</td>
<td>1992</td>
<td>(Maia et al., 1995)</td>
</tr>
<tr>
<td>Pumps (k$ /yr)</td>
<td>$0.73 W^{0.43}$</td>
<td>1992</td>
<td>(Maia et al., 1995)</td>
</tr>
<tr>
<td>Gas turbine (k$ /kW)</td>
<td>$0.273$</td>
<td>1992</td>
<td>(ASME, 1992-93)</td>
</tr>
<tr>
<td>Heat recovery exchanger (k$):</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- economisers</td>
<td>$C = 2.2 A^{0.5}$</td>
<td>1986</td>
<td>(Wells and Rose, 1986)</td>
</tr>
<tr>
<td>- evaporators</td>
<td>$C = 3.3 A^{0.5}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- superheaters</td>
<td>$C = 2.75 A^{0.5}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
while others for the installed cost of equipment. For units whose purchase cost was available installation factors were investigated and are presented in next section, so installed costs at year 1997 for all unit operations were finally used in the optimisation and synthesis problems.

In table E.2 the cost for steam turbines was in tabular form in (Maia et al., 1995), but correlated to get the expression shown.

### E.3 Installation factors

The installation factors for the equipments whose purchase cost was available are presented in Table E.3. Purchase cost times the installation factor gives the equipment installed cost used in our objective functions.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Installation factor (Ulrich, 1984)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air-cooled HX</td>
<td>2.0</td>
</tr>
<tr>
<td>Gas turbine</td>
<td>3.5</td>
</tr>
<tr>
<td>Heat recovery exchanger</td>
<td>1.8</td>
</tr>
</tbody>
</table>
References


REFERENCES


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