OPTI_ENERGY
Summer School: *Optimization of Energy Systems and Processes*

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Topic

METHODS OF ENERGY SYSTEMS OPTIMIZATION

by

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1. INTRODUCTION

In many fields of science and technology (the physical sciences, engineering, economics) the question is often posed: "what is the best way to achieve a specified goal?" For energy systems, in particular, this question may be expressed in several ways, including the following:

- Given the energy needs, what is the best type of energy system to be used?
- What is the best system configuration (components and their interconnections)?
- What are the best technical characteristics of each component (dimensions, material, capacity, etc.)?
- What are the best flow rates, pressures and temperatures of the various working fluids?
- What is the best operating point of the system at each instant of time?

When a number of plants are available to serve a certain region, questions such as the following arise:

- Which plants should be operated, and at what load under certain conditions?
- How should the operation and maintenance of each plant be scheduled in time?

A rational answer to these types of questions can be given by a systematic procedure, which is called *optimization.*

Methods appropriate for optimization of energy systems are presented in brief in this lecture. For a thorough knowledge of the subject, a study of the relevant literature is necessary.

The need for optimization

Energy systems in more or less complex forms have been built and operated since the 18th century. In a conventional design procedure, the aim is to reach a workable system, i.e a system that performs the assigned task within the imposed constraints. However, in general, there will be more than one workable design; and, in fact, there may be any number of better designs that the conventional procedure may not identify. The role of optimization is to reveal the best (under certain criteria and constraints) design and the best operational point of the system automatically, with no need for the designer to study and evaluate one by one the multitude of possible variations.

The following aspects show the necessity of applying optimization procedures in the design and operation of energy systems:

- Increasing the quality and capacity of the plants while reducing costs in order to be competitive.
- Fulfilling ever increasing specification as well as considering reliability and safety, observing strict pollution regulations, and saving energy and material resources.
- Saving time and increasing the designer's creativity.

2. DEFINITION OF OPTIMIZATION

A goal called an *objective function* is specified and is expressed as a mathematical function of certain variables. Then, optimization could be defined as follows:

Optimization is the process of finding the conditions, i.e. the values of variables, that give the minimum (or maximum) of the objective function.

In the literature on energy systems, the word "optimization" is often used in cases where the proper word is "improvement." The two words do not have the same meaning and care should be exercised in their use.

3. LEVELS OF OPTIMIZATION OF ENERGY SYSTEMS

The questions posed in the Introduction reveal that optimization of an energy system can be considered at three levels:

A. *Synthesis optimization.* The term "synthesis" implies the components that appear in a system and their interconnections. After the synthesis of a system has been successfully composed, the flow diagram of the system can be drawn.

B. *Design optimization.* The word "design" here is used to imply the technical characteristics (specifications) of the components and the properties of the substances entering and exiting each component at the nominal load of the system. The nominal load is usually called the "design point" of the system. One may argue that design includes synthesis too. However in order to distinguish the various levels of optimization and due to the lack of a better term, the word "design" will be used with the particular meaning given here.

C. *Operation optimization.* For a given system (i.e. one in which the synthesis and design are known) under specified conditions, the optimal operating point is requested, as it is defined by the operating properties of components and substances in the system (speed of revolution, power output, mass flow rates, pressures, temperatures, composition of fluids, etc.).

Of course if complete optimization is the goal, each level cannot be considered in complete isolation from the others. Consequently, the complete optimization problem can be stated by the following question:

What is the synthesis of the system, the design characteristics of the components and the operating strategy that lead to an overall optimum?

The degree of freedom increases further if the task of the system (i.e. its production rates) is not pre-specified but is to be determined by the optimization procedure. Time-dependent optimization adds one more dimension, which increases the complexity of the problem.

4. FORMULATION OF THE OPTIMIZATION PROBLEM

4.1 Mathematical Statement of the Optimization Problem

The general optimization problem consists of a determination of the extremum (minimum or maximum) of an objective function under certain constraints. It is usually stated mathematically as follows:

$$\underset{\mathbf{x}}{\text{minimize}}\ f(\mathbf{x}) \tag{4.1}$$

with respect to $$\mathbf{x} = (x_1, x_2, \ldots, x_n) \tag{4.2}$$

subject to the constraints

$$h_i(\mathbf{x}) = 0 \qquad i = 1, 2, \ldots, m \tag{4.3}$$

$$g_j(\mathbf{x}) \leq 0 \qquad j = 1, 2, \ldots, p \tag{4.4}$$

where

- $\mathbf{x}$ set of all the independent variables,
- h_i equality constraint functions ('strong' constraints), which constitute the simulation model of the system and are derived by an analysis of the system (energetic, exergetic, economic, etc.),
- g_j inequality constraint functions ('weak' constraints) corresponding to design and operation limits, state regulations, safety requirements, etc.

It is often helpful to arrange the independent variables into three sets:

$$\mathbf{x} \equiv (\mathbf{v}, \mathbf{w}, \mathbf{z}) \tag{4.5}$$

where

- $\mathbf{v}$ set of independent variables for operation optimization (load factors of components, mass flow rates, pressures and temperatures of streams, etc.),
- $\mathbf{w}$ set of independent variables for design optimization (nominal capacities of components, mass flow rates, pressures and temperatures of streams, etc.),
- $\mathbf{z}$ set of independent variables for synthesis optimization; there is only one variable of this type for each component, indicating whether the component exists in the optimal configuration or not; it may be a binary (0 or 1), an integer, or a continuous variable such as the rated power of a component, with a zero value indicating the non-existence of a component in the final configuration.

Then, Eq. (4.1) is written

$$\underset{\mathbf{v},\mathbf{w},\mathbf{z}}{\text{minimize}}\ f(\mathbf{v}, \mathbf{w}, \mathbf{z}) \tag{4.1$'$}$$

For a given synthesis (structure) of the system, i.e. for given $\mathbf{z}$, the problem becomes one of design and operation optimization:

$$\underset{\mathbf{v},\mathbf{w}}{\text{minimize}}\ f_d(\mathbf{v}, \mathbf{w}) \tag{4.1$_d$}$$

Furthermore, if the system is completely specified (both $\mathbf{z}$ and $\mathbf{w}$ are given), then an operation optimization problem is formulated:

$$\underset{\mathbf{v}}{\text{minimize}}\ f_{op}(\mathbf{v}) \tag{4.1$_{op}$}$$

Maximization is also covered by Eq. (4.1), since:

$$\min f(\mathbf{x}) = \max \{- f(\mathbf{x})\} \tag{4.6}$$

4.2 Objective Functions

The decision regarding which criterion is to be optimized is of crucial importance and the answer depends on the particular application: for example, in an aircraft or space vehicle, it may be the minimum weight of the system; in an automobile, it may be the minimum size of the system; in a stationary power plant it may be the minimum life cycle cost (LCC) of the system. Examples of other objective functions for energy systems include: maximization of efficiency, minimization of fuel consumption, minimization of exergy destruction, maximization of the net power density, minimization of emitted pollutants, maximization of the internal rate of return (IRR), minimization of the payback period (PBP), etc. Some of these are pure technical objectives, while the rest are (thermo)economic objectives.

In a complex world, a single objective may result in a system that does not satisfy other requirements. Consequently, the final design may deviate from, e.g., the least cost one, in order to take environmental, social, aesthetic or other aspects into consideration. Methods have been developed under the name "multiobjective optimization," which attempt to take two or more objectives into consideration simultaneously. The optimum point they reach does not satisfy each objective in isolation but it corresponds to a compromise, often subjective, of the various objectives. Multi-objective optimization can also be written in the form of Eq. (4.1), but only if the various objectives are combined into one objective function by means of weighting factors.

4.3 Independent Variables

Each component and the system as a whole is defined by a set of quantities. Certain of those are fixed by external conditions (e.g., environmental pressure and temperature, fuel price) and are called *parameters*. The remaining are variables, i.e. their value may change during the optimization procedure. Those variables, the values of which do not depend on other variables or parameters, are called *independent variables*. The rest can be determined by the solution of the system of equality constraints and they are called *dependent variables*. The number of dependent variables is equal to the number of equality constraints. Thus, the task of the optimization procedure is to determine the values of the independent variables $\mathbf{x}$. Of course, if the number of equality constraints is higher than the number of all the variables, then the problem is over-specified and there is no room for optimization.

4.4 Equality and Inequality Constraints

The functions appearing in Eqs. (4.3) and (4.4) are expressions involving design characteristics and operating parameters or variables of the components as well as the system as a whole. For example, the required mass flow rate of steam in a steam turbine is given as a function of the power output and the properties of steam at the inlet and outlet of the turbine. On the other hand, the safety and operability of the system impose inequality constraints such as the following: speed of revolution not higher than a certain limit; quality (dryness) of steam at the exit of the steam turbine not lower than a certain limit, etc.

The set of equality and inequality constraints is derived by an analysis of the system and constitutes the mathematical model of the system. Models may initially be developed at the level of each component, which are then integrated to form the model of the whole system.

A word of caution: describing reality by mathematics is not an easy task and it is often accompanied by simplifying assumptions, which introduce inaccuracies. This is mentioned not in order to deter one from applying modeling and optimization techniques, but to make it clear that the solution (synthesis, design or operation point) reached is optimal only under the assumptions made in modeling the system; and it is as close to the real optimum as any discrepancies between model and reality allow. However, most probably, if a care has been taken, it is closer than a decision based only on past experience or similar preceding designs.

5 MATHEMATICAL METHODS FOR SOLUTION OF THE OPTIMIZATION PROBLEM

In spite of their apparent generality, there is no single method available for solving efficiently all the optimization problems stated by Eqs. (4.1) – (4.4). A number of methods have been developed for solving different types of optimization problems. They are known as *mathematical programming methods* and they are usually available in the form of a mathematical programming algorithm.

5.1 Classes of Mathematical Optimization Methods

Optimization problems and the techniques developed for their solution can be classified in several ways, depending on the criterion. The classification is very useful from the computational point of view, because there are many special methods available for the efficient solution of particular classes of problems.

5.1.1 Constrained and unconstrained programming

Any optimization problem can be classified as constrained or unconstrained, depending on whether or not constraints exist in the problem.

5.1.2 Search and calculus (or gradient) methods

A *search method* uses values of the objective function in order to locate the optimum point, with no use of derivatives. On the contrary, *calculus methods* use first and (some of them) second derivatives; this is why they are called also *gradient methods*. Search methods calculate the values of the objective function at a number of combinations of values of the independent variables and seek for the optimum point. The search may be random or systematic, the second one usually being more efficient.

In general, gradient methods converge faster than the search methods, but in certain cases they may not converge at all.

If the objective function is continuous, by applying a search method the exact optimum can only be approached, not reached, by a finite number of trials, because only discrete points are examined. However, the region, in which the optimum point is located, can be reduced to a satisfactorily small size at the end of the procedure. On the other hand, there are problems for which search methods may be superior to calculus methods, as for example in optimization of systems with components available only in finite sizes.

5.1.3 Linear, nonlinear, geometric and quadratic programming

This classification is based on the nature of the equations involved. If the objective function and all the constraints are linear functions of the independent variables, then a linear programming (LP) problem is at hand. If at least one of the functions (no matter whether it is the objective function or one of the constraint functions) is nonlinear, then the problem is a nonlinear programming (NLP) problem.

A geometric programming (GMP) problem is one in which the objective function and the constraints are expressed as posynomials in **x**. A function f(**x**) is called a *posynomial*, if it has the form

$$f(\mathbf{x}) = c_1 x_1^{a_{11}} x_2^{a_{12}} \ldots x_n^{a_{1n}} + \ldots + c_N x_1^{a_{N1}} x_2^{a_{N2}} \ldots x_n^{a_{Nn}} \tag{5.1}$$

where c_i and a_{ij} are constants and $c_i > 0$, $x_j > 0$.

A quadratic programming (QP) problem is a nonlinear programming problem with a quadratic objective function and linear constraints.

5.1.4 Integer- and real-valued programming

This classification is based on the values permitted for the independent variables. If some or all of the independent variables of an optimization problem are restricted to take on only integer (or discrete) values, then the problem is called an *integer programming* (IP) problem. If all the independent variables are permitted to take any real value, then the optimization problem is called a *real-valued programming* problem.

The existence of integer variables in linear and nonlinear programming problems leads to *mixed integer linear programming* (MILP) and *mixed integer nonlinear programming* (MINLP) problems, respectively.

5.1.5 Deterministic and stochastic Programming

If some or all of the prespecified parameters and/or independent variables are probabilistic (nondeterministic or stochastic), then the optimization problem is *a stochastic programming problem*. Otherwise, it is a *deterministic programming problem*.

5.1.6 Separable programming

A function f(**x**), **x** = (x_1, x_2, …, x_n), is called *separable* if it can be expressed as the sum of n single-variable functions:

$$f(\mathbf{x}) = \sum_{i=1}^{n} f_i(x_i) \tag{5.2}$$

A separable programming problem is one in which the objective function and the constraints are separable functions.

5.1.7 Single and multiobjective programming

Depending on the number of objective functions, optimization problems can be classified as *single-objective* or *multiobjective* programming problems. In most of the problems there is no single point **x*** that satisfies all the objectives simultaneously. Therefore, there is usually need of a compromise, often subjective.

5.1.8 Dynamic programming and calculus of variations

Dynamic programming (DP) or calculus of variations (COV) is applied when an optimal function rather than an optimal point is sought. The calculus of variations seeks a function that optimizes an integral; in a single variable, the problem is stated as

$$\min_{y} I = \int_{x_1}^{x_2} F(x, y, y', y'')\, dx \tag{5.3}$$

where y=y(x) is the function sought, F is a known function and $y' = \frac{dy}{dx}$, $y'' = \frac{d^2y}{dx^2}$

Dynamic programming is applicable to staged processes or to continuous functions that can be approximated by staged processes. Thus, the decision variables are sought for which, for a specified input to stage n and a specified output from stage 1, the summation

$$\sum_{i=1}^{n} f_i(y)$$

is optimum.

COV and DP are both methods to determine y(x). Which method is precise and which is an approximation depends on the problem. If, for example, the velocity of a vehicle is continuously adjusted during a trip to minimize the total fuel consumption, COV is a precise representation and DP is an approximation (since it would represent the varying speed as a series of steps). If, however, the problem were to optimize the sizes of a series of heat exchangers, DP would be the precise method and COV an approximation.

5.1.9 Genetic Algorithms

Genetic Algorithms (GAs) have been developed by J. Holland in an attempt to simulate growth and decay of living organisms in a natural environment. Even though originally designed as simulators, GAs proved to be a robust optimization technique. Philosophically GAs are based on the concepts of biological evolution (natural genetics and natural selection) and Darwin's theory of survival of the fittest. The basic elements of natural genetics, i.e., reproduction, crossover and mutation, are used in the genetic search procedure. The main characteristics of the GAs, which highlight also their differences from the traditional methods of optimization, are the following:

1. A population of points (instead of a single point) inside the optimization space, selected randomly, is used to start the procedure. Since several points are used as candidate solutions, GAs are less likely to be trapped at a local optimum.
2. The GAs use only the values of the objective function. The derivatives are not used.
3. In GAs the decision variables are represented as strings of binary variables that correspond to the chromosomes in natural genetics. Any type of variables, either discrete (e.g. integers) or continuous, can be handled. For continuous variables, the string can be selected so that the desired resolution is achieved.
4. The value of the objective function of each string in a population plays the role of fitness in natural genetics.
5. A new population is generated (reproduction) by applying randomized crossover and mutation on the old one. The value of the objective function is used so that "weak" strings are dropped out, while "strong" strings give more offsprings in the new population. The procedure is repeated until no further improvement is achieved.

The aforementioned show that GAs are appropriate for problems with mixed discrete-continuous variables and discontinuous and non-convex decision spaces. Furthermore, in most cases they have a high probability in finding the global optimum.

5.1.10 Simulated Annealing

Simulated annealing is a combinatorial optimization technique based on random evaluation of the objective function. The name of the method is derived from the thermal annealing of the solids. The method proceeds as follows. Let $\mathbf{x}_i$ be the current point (vector). Random moves are made along each coordinate, in turn. The new coordinate values are uniformly distributed around the corresponding coordinate of $\mathbf{x}_i$. One half of these intervals along the coordinates are stored as the step vector $\mathbf{s}_i$. A candidate decision vector $\mathbf{x}_i$ is accepted or rejected according to a criterion known as the *metropolis criterion*:

If $\Delta f \leq 0$, accept the new point and set $\mathbf{x}_{i+1} = \mathbf{x}$. Otherwise, accept the new point with a probability of

$$P(\Delta f) = e^{-\Delta f / kT} \tag{5.4}$$

where $\Delta f = f(\mathbf{x}_{i+1}) - f(\mathbf{x})$, k is a scaling factor called *Boltzmann's constant*, and T is a parameter called *temperature*.

The value of k influences the convergence characteristics of the method. Various *cooling* schedules, defining the variations of k and T from one iteration to the other have been studied. A high initial temperature T_0 is selected and then it is gradually reduced. Although the method requires a large number of function evaluations to find the optimum solution, it will find the global optimum with high probability, even for ill-conditioned functions with numerous local minima.

5.1.11 Other methods

In addition to the aforementioned, there are optimization techniques based on neural networks, as well as methods for optimization of fuzzy systems. However, their description is beyond the limits of this lecture.

5.2 Basic Principles of Calculus Methods

The classical methods of optimization are analytical and make use of differential calculus to locate the optimum points. They are applicable on problems with continuous and differentiable functions. Many practical problems either do not satisfy these requirements or they are expressed by a system of equations, which cannot be solved analytically. In such cases there is need of numerical methods for their solution. A study of the calculus methods of optimization is useful not only for the cases these methods are applicable, but also because they form the basis for most of the numerical optimization techniques. Only the basic principles are presented in the following.

5.2.1 Single-variable optimization

A function f(x) is said to have a *relative* or *local* minimum at x* if $f(x^*) \leq f(x^* + \varepsilon)$ for all sufficiently small positive and negative values of ε. A function f(x) is said to have an *absolute* or *global* minimum at x* if $f(x^*) \leq f(x)$ for all x in the domain over which f(x) is defined. Similar definitions are applicable for points where f(x) is maximized. A function with more than one minimum or maximum point is called *multimodal*. Figure 1 shows examples of local and global optimum points.

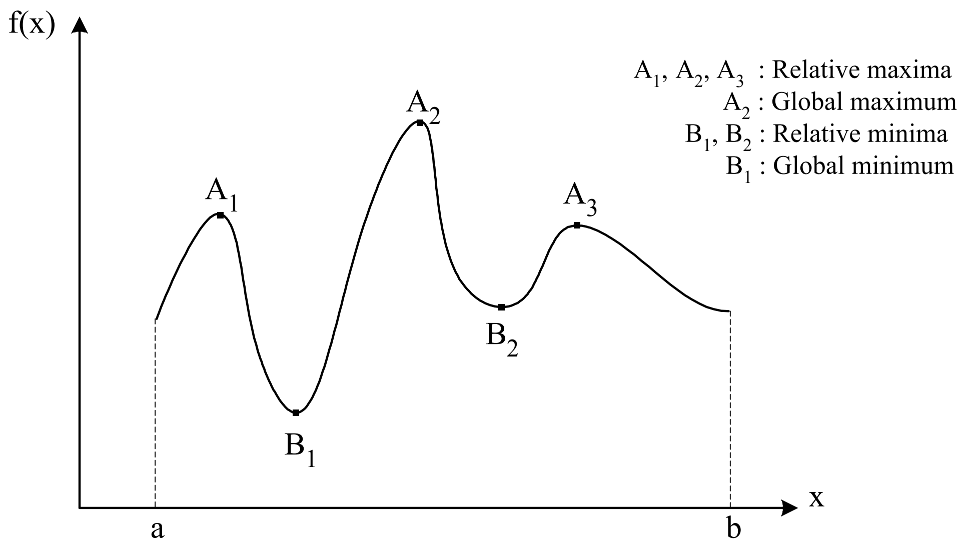

Fig. 5.1. Local and global optimum points.

Theorem 1: Necessary condition.

Necessary condition for x* to be a local minimum or maximum of f on the open interval (a, b) is that

$$f'(x^*) = 0 \tag{5.5}$$

The condition is necessary in the sense that, if it is not satisfied, x* is neither a minimum nor a maximum, but if it satisfied, there is no guarantee that x* is a minimum or maximum; it may be an inflection point (Fig. 5.2). A point x*, where Eq. (5.5) is satisfied, is called *stationary point* (Fig. 5.2).

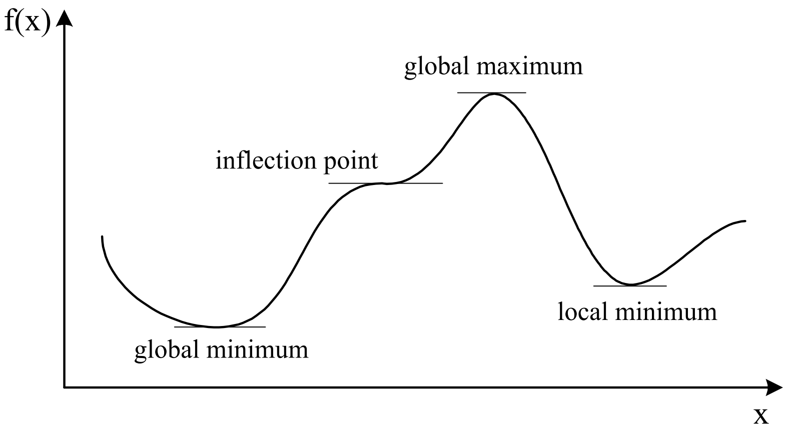

Fig. 5.2. Stationary points.

Theorem 2: Sufficient condition.

Let all the derivatives of a function up to order (n-1) be equal to zero and that the *n*th order derivative is nonzero:

$$f'(x^*) = f''(x^*) = \ldots = f^{(n-1)}(x^*) = 0\,, \qquad f^{(n)}(x^*) \neq 0 \tag{5.6}$$

where

$$f^{(n)}(x) = \frac{d^n f(x)}{dx^n} \tag{5.7}$$

If n is odd, then x* is a point of inflection.
If n is even, then x* is a local optimum. Moreover:

If $f^{(n)}(x^*) > 0$, then x* is a local minimum.

If $f^{(n)}(x^*) < 0$, then x* is a local maximum.

Notes.

1. The end points of the interval [a, b] are not covered by the preceding theorems, i.e., points x=a and x=b may be optimum points even if the necessary and sufficient conditions are not satisfied.

2. Theorems 1 and 2 may not hold for optimum points where the derivatives are not uniquely defined.

Example

In a two-stage compressor the gas leaving the first stage passes through a heat exchanger where it is cooled down to its initial temperature T_1, and then it enters the second stage. If the total pressure ratio is r, determine the pressure ratio r_1 of the first stage that minimizes the input work to the compressor. For simplicity, assume isentropic compression in both stages.

<u>Solution.</u> The compression work per unit mass of gas is given by the equation

$$w = c_p T_1 \left[r_1^{\gamma} + \left(\frac{r}{r_1} \right)^{\gamma} - 2 \right]$$

where $\gamma = (k-1)/k$

- k specific heat ratio: $k = c_p / c_v$
- c_p specific heat at constant pressure,
- c_v specific heat at constant volume.

The necessary condition to minimize w is: $dw/dr_1 = 0$. Since c_p and T_1 are constant, the condition is equivalent to $df/dr_1 = 0$, where

$$f \equiv \frac{w}{c_p T_1} = r_1^{\gamma} + \left(\frac{r}{r_1} \right)^{\gamma} - 2$$

The condition $$\frac{df}{dr_1} = \gamma r_1^{\gamma-1} - r^{\gamma} \gamma r_1^{-\gamma-1} = 0$$

results in $$r_1^* = \sqrt{r}$$

The second derivative of f is $$\frac{d^2 f}{dr_1^2} = \gamma(\gamma-1) r_1^{\gamma-2} + \gamma(\gamma+1) r^{\gamma} r_1^{-\gamma-2} > 0$$

i.e., it is positive for every value of r_1, including r_1^* (note that r>1, r_1>1). Consequently, r_1^* is a minimum point of f and w.

5.2.2 Multi-variable optimization with no constraints

The necessary and sufficient conditions are extended to optimization problems with many decision variables, initially with no constraints. Before stating the theorems (optimality conditions), there is need of certain definitions.

Definitions

The first derivatives of a function f(**x**) of n variables are written as

$$\nabla f(\mathbf{x}) = \left(\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_n} \right) \tag{5.8}$$

where $\nabla f(\mathbf{x})$ is treated as an n-component column vector (or matrix).

The matrix of second partial derivatives of f(**x**), which is called *Hessian matrix*, is written

$$F(\mathbf{x}) \equiv H_f(\mathbf{x}) \equiv \nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{5.9}$$

Principal minor of order k of a symmetric matrix n×n is the matrix, which is derived if the last n-k lines and columns of the initial matrix are deleted. Every n×n matrix has n principal minors.

If A is an n×n matrix and **z** is an n-component vector, i.e., $\mathbf{z}^T = (z_1, z_2, \ldots, z_n)$, then matrix A is

positive definite	if for every **z**≠0	it is	$\mathbf{z}^T A \mathbf{z} > 0$
positive semidefinite	if for every **z**≠0	it is	$\mathbf{z}^T A \mathbf{z} \geq 0$
negative definite	if for every **z**≠0	it is	$\mathbf{z}^T A \mathbf{z} < 0$
negative semidefinite	if for every **z**≠0	it is	$\mathbf{z}^T A \mathbf{z} \leq 0$
indefinite	if for some **z**	it is	$\mathbf{z}^T A \mathbf{z} > 0$
	and for other **z**	it is	$\mathbf{z}^T A \mathbf{z} < 0$

A practical rule to determine the type of a matrix A is the following. The principal minor of order k is given the symbol $|A_k|$. Matrix A is

positive definite	if for every k = 1, 2, …, n	it is	$\lvert A_k \rvert > 0$
positive semidefinite	if for every k = 1, 2, …, n	it is	$\lvert A_k \rvert \geq 0$
negative definite	if the value of $\lvert A_k \rvert$	has the sign $(-1)^k$	
negative semidefinite	if the value of $\lvert A_k \rvert$	has the sign $(-1)^k$ or it is zero.	

Theorem 3: Necessary conditions.

Necessary conditions for an interior point **x*** of the n-dimensional space $\Omega \subset R^n$ to be a local minimum or maximum of f(**x**) is that

$$\nabla f\left(\mathbf{x}^*\right)=0 \tag{5.10}$$

and

$$\nabla^2 f\left(\mathbf{x}^*\right) \text{ is positive semidefinite.} \tag{5.11}$$

If Eq. (5.10) is satisfied, then **x*** is a minimum, maximum or saddle point. A saddle point is the extension of the inflection point to the n-dimensional space. A visualization of the saddle point in the two-dimensional space (n=0) is given in Fig. 5.3.

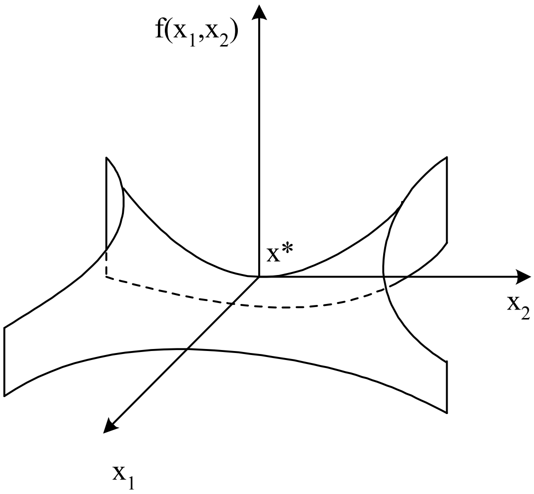

Fig. 5.3. Saddle point: **x***.

Theorem 4: Sufficient conditions.

If an interior point x* of the space $\Omega \subset R^n$ satisfies Eq. (5.10) and $\nabla^2 f\left(\mathbf{x}^*\right)$ is positive (or negative) definite, then x* is a local minimum (or maximum) of f (**x**).

5.2.3 Multi-variable optimization with equality constraints (Lagrange theory)

The optimization problem is stated for this case as follows:

$$\min_{\mathbf{x}} f(\mathbf{x}) \tag{5.12a}$$

subject to

$$h_i(\mathbf{x})=0, \qquad i=1,2,\ldots,m \tag{5.12b}$$

It is converted to a problem with no constraints by means of the *Lagrangian function*:

$$L(\mathbf{x},\boldsymbol{\lambda})=f(\mathbf{x})+\sum_{i=1}^{m}\lambda_i\, h_i(\mathbf{x}) \tag{5.13}$$

where $\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\ldots,\lambda_m)$ are the *Lagrange multipliers*.

The necessary conditions are:

$$\nabla_{\mathbf{x}} \mathrm{L}\left(\mathbf{x}^*, \boldsymbol{\lambda}^*\right) = 0 \tag{5.14a}$$

$$\nabla_{\boldsymbol{\lambda}} \mathrm{L}\left(\mathbf{x}^*, \boldsymbol{\lambda}^*\right) = 0 \tag{5.14b}$$

Equation (5.14b) is, in fact, a restatement of the equality constraints, Eq. (5.12b). The system of Eq. (5.14) consists of n+m equations, and its solution gives the values of the n+m unknown **x*** and **λ***.

The sufficient conditions are stated in a similar way as in Theorem 4, where $\nabla_{\mathbf{x}}^2 \mathrm{L}\left(\mathbf{x}^*, \boldsymbol{\lambda}^*\right)$ is used, instead of $\nabla^2 \mathrm{f}\left(\mathbf{x}^*\right)$.

5.2.4 The general optimization problem (Kuhn - Tucker theory)

Lagrange's theory has been extended by Kuhn and Tucker in order to solve problems with both equality and inequality constraints, as stated by Eqs. (4.1) – (4.4).

Definitions

A point **x*** which satisfies all the equality and inequality constraints is called a *feasible point*.

A point **x*** which satisfies the equality constraints $\mathrm{h}_\mathrm{i}(\mathbf{x}) = 0, \quad \mathrm{i} = 1, 2, \ldots, \mathrm{m}$, is called a *regular point* of the constraints, if the gradient vectors $\nabla \mathrm{h}_\mathrm{i}\left(\mathbf{x}^*\right), \quad \mathrm{i} = 1, 2, \ldots, \mathrm{m}$, are linearly independent.

An inequality constraint $\mathrm{g}_\mathrm{j}\left(\mathbf{x}^*\right) \le 0$ is called *active* at the point **x***, if it is $\mathrm{g}_\mathrm{j}\left(\mathbf{x}^*\right) = 0$.

A point $\mathbf{x}^* \in \Omega$ is called *strict local minimum* of f(**x**) in Ω, if there exists an $\varepsilon \ge 0$ such that f(**x**) ≥ f(**x***) for every $\mathbf{x}^* \in \Omega$ in a distance ε from **x*** (i.e., $\left|\mathbf{x} - \mathbf{x}^*\right| < \varepsilon$).

Kuhn – Tucker conditions (necessary conditions)

Let **x*** be a local minimum of the optimization problem (4.1) – (4.4) and a regular point of the equality and active inequality constraints. Then, there exists a vector $\boldsymbol{\lambda} \in \mathrm{R}^\mathrm{m}$ and a vector $\boldsymbol{\mu} \in \mathrm{R}^\mathrm{p}$, with $\boldsymbol{\mu} \ge 0$, such that

$$\nabla \mathrm{f}\left(\mathbf{x}^*\right) + \boldsymbol{\lambda} \cdot \nabla \mathbf{h}\left(\mathbf{x}^*\right) + \boldsymbol{\mu} \cdot \nabla \mathbf{g}\left(\mathbf{x}^*\right) = 0 \tag{5.15a}$$

$$\boldsymbol{\mu} \cdot \mathbf{g}\left(\mathbf{x}^*\right) = 0 \tag{5.15b}$$

where

$$\mathbf{h} = \left(\mathrm{h}_1, \mathrm{h}_2, \ldots, \mathrm{h}_\mathrm{m}\right)$$
$$\mathbf{g} = \left(\mathrm{g}_1, \mathrm{g}_2, \ldots, \mathrm{g}_\mathrm{p}\right).$$

Sufficient conditions

Sufficient conditions that a feasible point **x*** be a strict local minimum of the optimization problem is that there exist $\boldsymbol{\lambda} \in R^m, \boldsymbol{\mu} \in R^p, \boldsymbol{\mu} \geq 0$, such that Eqs. (5.15) are satisfied and the Hessian matrix

$$\mathsf{L}\left(\mathbf{x}^*\right) = F\left(\mathbf{x}^*\right) + \sum_{i=1}^{m} \lambda_i H_i\left(\mathbf{x}^*\right) + \sum_{j=1}^{p} \mu_j G_j\left(\mathbf{x}^*\right) \tag{5.16}$$

is positive definite at every point **z** of the subspace

$$M = \left\{\mathbf{z}: \quad \nabla\mathbf{h}(\mathbf{x}^*)\cdot\mathbf{z} = 0, \quad \nabla g_j(\mathbf{x}^*)\cdot\mathbf{z} = 0 \quad \forall j \in J\right\} \tag{5.17a}$$

where

$$J = \left\{j: \; g_j\left(\mathbf{x}^*\right) = 0, \quad \mu_j > 0\right\} \tag{5.17b}$$

i.e.

$$\mathbf{z}^T \, \mathsf{L}\left(\mathbf{x}^*\right)\mathbf{z} > 0 \tag{5.18}$$

5.3 Nonlinear Programming Methods

Application of the theory presented in Subsection 5.3 leads to a system of equations (obtained by the necessary conditions) with respect to **x**. The solution of this system gives the optimum point **x***. However in real-world problems, the analytic solution is often difficult or even impossible. To overcome these difficulties, numerical methods have been and continue being developed. Many of these do not use the necessary conditions, but they exploit certain properties of the functions.

Many optimization methods have been developed throughout the years. Only five of these will be presented in brief in the following, which have been successful in solving problems of energy systems optimization. All five methods belong to "classical" mathematical programming, i.e. they are not based on genetic algorithms, simulated annealing or other evolutionary techniques. For more complete information, the interested reader may study the bibliography [e.g., Luenberger 1973, Reklaitis et al. 1983, Rao 1996, Papalambros and Wilde 2000].

It is clarified that linear programming methods are not presented here, because most of the energy systems optimization problems are nonlinear.

5.3.1 Single-variable nonlinear programming methods

Golden section search

The method uses values of the function with no need of derivatives.

Before applying the method, there is need to determine the interval [a, b], where a minimum point x* exists. This can be done by a random search or, more systematically, by the Swann method [Reklaitis et al. 1983]. Then, the optimum point is determined as follows.

The length of the initial interval containing the optimum point is

$$L_0 = b - a$$

The function f(x) is evaluated at the two points:

$$x_1 = \alpha + (1 - \tau)\, L_0 \tag{5.19a}$$

$$x_2 = \alpha + \tau\, L_0 \tag{5.19b}$$

where τ is the golden section ratio, obtained as the positive solution of the equation

$$\frac{1-\tau}{\tau} = \frac{\tau}{1} \qquad \Rightarrow \qquad 1 - \tau = \tau^2 \tag{5.20}$$

i.e.:

$$\tau = \frac{-1 + \sqrt{5}}{2} = 0{,}61803...$$

If $f(x_1) < f(x_2)$, then x^* is located in the interval (a, x_2).
If $f(x_1) \geq f(x_2)$, then x^* is located in the interval (x_1, b).

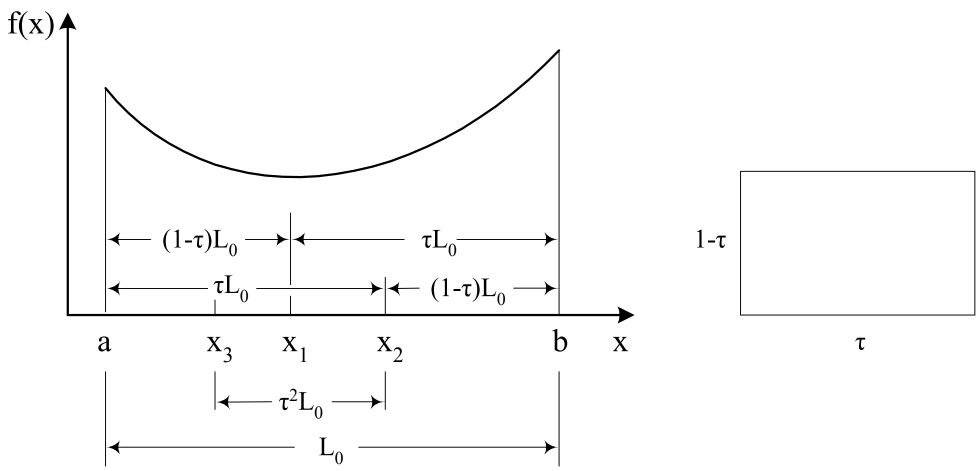

Fig. 5.4. Golden section search.

Whichever the new interval is, its length is

$$L_1 = x_2 - a = b - x_1 = \tau\, L_0$$

The procedure is repeated. After N iterations, the *interval of uncertainty*, i.e. the interval containing the optimum point, has a length of

$$L_N = \tau^N\, L_0 \tag{5.21}$$

The iterations are terminated when one or more of the convergence criteria are satisfied:

(i) $N \geq N_{max}$ (large number of iterations),

(ii) $L_N \leq \varepsilon_1$ (sufficiently small interval of uncertainty),

(iii) $\left|f\left(x_{N+1}\right) - f\left(x_N\right)\right| \leq \varepsilon_2$ (negligible improvement in the value of the objective function from one iteration to the other).

If a satisfactory interval of uncertainty, L_N, is specified, then the number of iterations needed is determined from the solution of Eq. (5.21) with respect to N:

$$N = \frac{\ell n\left(L_N / L_0\right)}{\ell n\, \tau} \tag{5.22}$$

Newton – Raphson method

The method requires that f(x) is twice differentiable. It begins with a point x_1 that is an initial estimate of the stationary point, i.e. of the solution of the equation $f'(x) = 0$. A linear approximation of the function $f'(x)$ is constructed, and the point at which the linear approximation becomes equal to zero (the straight line crosses the horizontal axis) is taken as the next trial point, x_2 (Fig. 5.5). Thus, the series of trial points is determined by the equation

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \tag{5.23}$$

which converges to x*, as shown in Fig. 5.5.

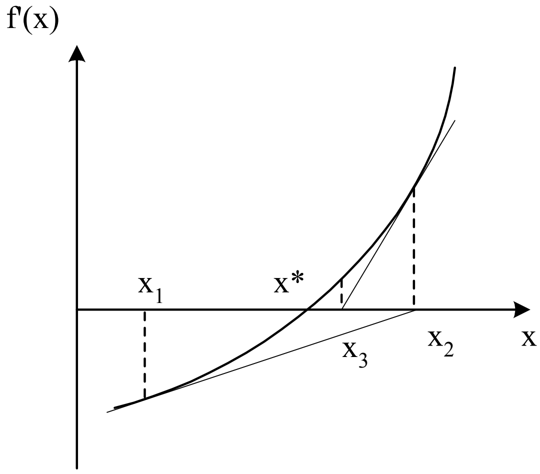

Fig. 5.5. Newton – Raphson method (convergence).

One or more of the following convergence criteria are used for termination of the procedure:

(i) $\left|f'\left(x_{k+1}\right)\right| \leq \varepsilon_1$

(ii) $\left|x_{k+1} - x_k\right| \leq \varepsilon_2$

(iii) $\left|f\left(x_{k+1}\right) - f\left(x_k\right)\right| \leq \varepsilon_3$

where $\varepsilon_1, \varepsilon_2, \varepsilon_3$ are sufficiently small numbers.

When it converges, the Newton – Raphson method is the fastest of all. However the form of $f'(x)$ and the starting point may make the procedure to diverge instead of converging to the stationary point. Such a case is illustrated in Fig. 5.6: if the starting point is to the right of x_0, then the successive approximations lead away from the stationary point x*.

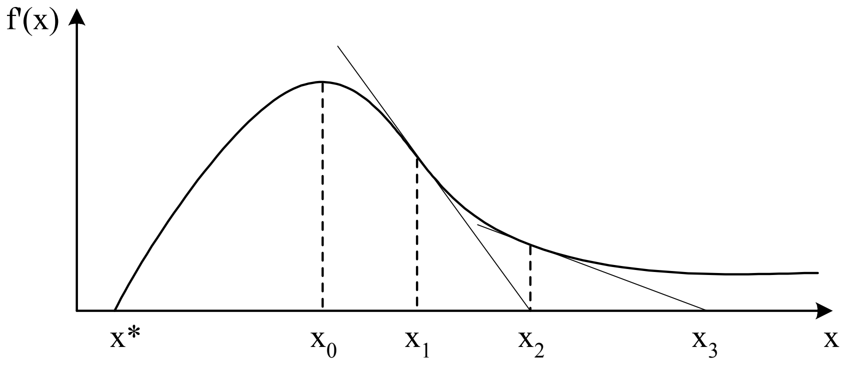

Fig. 5.6. Divergence of Newton – Raphson method.

One more disadvantage of the method is that, if the function $f'(x)$ is very flat, a point x_{k+1} may satisfy all the three aforementioned criteria of convergence and, consequently, the iterations are terminated, but the point x_{k+1} may still be far from the optimum x*.

Modified Regula Falsi method (MRF)

Two initial points a_0 and b_0 are determined such that f(x) is continuous on [a_0, b_0] and

$$f'(a_0) \cdot f'(b_0) < 0$$

Then it is
$$a_0 < x^* < b_0$$

The procedure is illustrated in Fig. 5.7 and consists of the following steps [Conte and de Boor, 1980]:

1. Set $\quad F = f'(a_0), \quad G = f'(b_0), \quad x_0 = a_0$

2. For n = 0, 1, 2,… until convergence

calculate
$$x_{n+1} = \frac{G\,a_n - F\,b_n}{G - F} \tag{5.24}$$

If $\quad f'(a_n) \cdot f'\left(x_{n+1}\right) \leq 0$, set

$$a_{n+1} = a_n, \quad b_{n+1} = x_{n+1}, \quad G = f'\left(x_{n+1}\right)$$

If also $f'\left(x_n\right) \cdot f'\left(x_{n+1}\right) > 0$, set $F = F/2$

If $f'\left(a_n\right) \cdot f'\left(x_{n+1}\right) > 0$, set

$$a_{n+1} = x_{n+1}, \quad b_{n+1} = b_n, \quad F = f'\left(x_{n+1}\right)$$

If also $f'\left(x_n\right) \cdot f'\left(x_{n+1}\right) > 0$, set $G = G/2$

The function $f'\left(x\right) = 0$ has a solution in the interval $[a_{n+1}, b_{n+1}]$.

The following criteria of convergence can be used:

(i) $\left|f'\left(x_{n+1}\right)\right| \le \varepsilon_1$

(ii) $\left|b_{n+1} - a_{n+1}\right| \le \varepsilon_2$

(iii) $\left|f\left(x_{n+1}\right) - f\left(x_n\right)\right| \le \varepsilon_3$

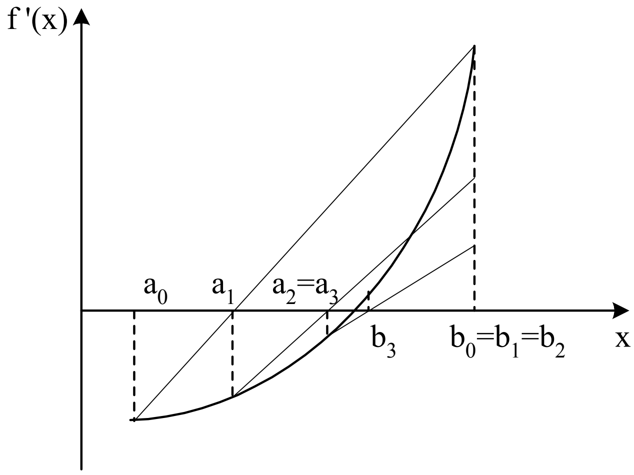

Fig. 5.7. Modified Regula Falsi method.

Advantages of the method are the guaranteed convergence and bracketing of the solution in a known and sufficiently small interval of uncertainty $[a_{n+1}, b_{n+1}]$.

5.3.2 Multi-variable nonlinear programming methods

Relatively simple optimization problems can be solved by one of the single-variable methods described in §5.3.1, which is applied on one direction after the other, in a cyclic approach. Such a procedure has been successful in optimization problems of energy systems with up to six independent variables and functions rather smooth. Even in these cases, however, it may be preferable (at least from the point of view of speed) to apply one of the many methods, which have been developed for multi-variable nonlinear optimization problems. Only the two most successful of these methods for energy systems optimization are described in brief in the following.

Generalized Reduced Gradient method (GRG)

The method is an extension of the *reduced gradient method* that was developed initially for solving problems with linear constraints only. It is based on the idea that, if an optimization problem has n independent variables $\mathbf{x}$ and m equality constraints, then, at least in theory, the system of m equations can be solved for m of the independent variables. Thus, the number of independent variables is reduced to n-m, the dimensionality of the optimization problem is decreased and the solution is facilitated.

In the GRG method, the optimization problem is initially stated as follows:

$$\min f(\mathbf{x}) \tag{5.25a}$$

subject to

$$h_j(\mathbf{x}) = 0, \qquad j = 1, 2, \ldots, m \tag{5.25b}$$

$$g_k(\mathbf{x}) \le 0, \qquad k = 1, 2, \ldots, p \tag{5.25c}$$

$$x_i^L \le x_i \le x_i^U, \qquad i = 1, 2, \ldots, n \tag{5.25d}$$

where x_i^L and x_i^U are the lower and upper limits of x_i. By adding a nonnegative slack variable to each of the inequality constraints, the problem can be stated as

$$\min f(\mathbf{x}) \tag{5.26a}$$

subject to

$$h_j(\mathbf{x}) = 0, \qquad j = 1, 2, \ldots, m \tag{5.26b}$$

$$g_k(\mathbf{x}) + x_{n+k} = 0, \qquad k = 1, 2, \ldots, p \tag{5.26c}$$

$$x_i^L \le x_i \le x_i^U, \qquad i = 1, 2, \ldots, n \tag{5.26d}$$

$$x_{n+k} \ge 0, \qquad k = 1, 2, \ldots, p \tag{5.26e}$$

The new problem has n+k variables and can be written in a general form as

$$\min f(\mathbf{x}) \tag{5.27a}$$

subject to

$$\varphi_j(\mathbf{x}) = 0, \qquad j = 1, 2, \ldots, m + p \tag{5.27b}$$

$$x_i^L \le x_i \le x_i^U, \qquad i = 1, 2, \ldots, n + p \tag{5.27c}$$

The lower and upper bounds on the slack variables x_i, (i = n+1, n+2, …, n+p), are taken as 0 and a large number (infinity), respectively.

Of the n+p variables, m+p can be evaluated by the solution of the system of equality constraints, Eq. (5.27b). For this purpose, the set of variables $\mathbf{x}$ is divided into two subsets:

$$(\mathbf{x}) = (\mathbf{y}, \mathbf{z}) \tag{5.28a}$$

$$(\mathbf{y}) = y_1, y_2, \ldots, y_{n-m} \tag{5.28b}$$

$$(\mathbf{z}) = z_1, z_2, \ldots, z_{m+p} \tag{5.28c}$$

where

- **y** *independent variables,*
- **z** *dependent variables*, i.e. they depend on the independent variables so, that the equality constraints, Eq. (5.27b) are satisfied.

The independent variables are called also *decision variables*. The dependent variables are called also *state variables*.

The *generalized reduced gradient*, $\mathbf{G}_R$, is defined for the problem (5.27) as:

$$\mathbf{G}_R \equiv \frac{d f(\mathbf{x})}{d \mathbf{y}} \tag{5.29}$$

It is known that a necessary condition for the existence of a minimum of an unconstrained function is that the components of the gradient (first derivatives) are zero. Similarly, a constrained function obtains its minimum value when the appropriate components of the reduced gradient are zero. In fact, the generalized reduced gradient $\mathbf{G}_R$ can be used to generate a search direction towards the optimum point. A complete mathematical description of the method and the algorithmic steps are presented in [Rao, 1996].

Sequential Quadratic Programming (SQP)

The sequential quadratic programming is one of the most recently developed and one of the best methods of optimization.

An optimization problem is called a problem of quadratic programming, if it consists of a quadratic objective function and linear constraints. It is stated as:

$$\begin{aligned} \min f(\mathbf{x}) &= \mathbf{C}\,\mathbf{x} + \mathbf{x}^T \mathbf{D}\,\mathbf{x} = \\ &= \sum_{j=1}^{n} c_j x_j + \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} x_i x_j \end{aligned} \tag{5.30a}$$

$$\mathbf{A}\,\mathbf{x} \le \mathbf{B} \tag{5.30b}$$

$$\mathbf{x} \ge 0 \tag{5.30c}$$

where

$$\mathbf{x} = [x_1, x_2, \ldots, x_n]$$

$$\mathbf{C} = [c_1, c_2, \ldots, c_n]$$

$$\mathbf{B} = [b_1, b_2, \ldots, b_m]$$

$$\mathbf{A} = \begin{bmatrix} a_{11}, a_{12}, \ldots, a_{1n} \\ a_{21}, a_{22}, \ldots, a_{2n} \\ \vdots \quad \vdots \quad \vdots \\ a_{m1}, a_{m2}, \ldots, a_{mn} \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} d_{11}, d_{12}, \ldots, d_{1n} \\ d_{21}, d_{22}, \ldots, d_{2n} \\ \vdots \quad \vdots \quad \vdots \\ d_{n1}, d_{n2}, \ldots, d_{nn} \end{bmatrix}$$

It is considered that **D** is positive definite (for minimization problems), and consequently f(**x**) is strictly convex. Furthermore, due to the linear constraints, the space of feasible solutions is convex, and consequently the local optimum is also global optimum. For the same reasons, the necessary optimality conditions are also sufficient.

For the solution of the problem, the inequality constraints are converted to equality constraints by means of slack variables, the Lagrangian function is formed, and the necessary conditions are written. Since the objective function is of second degree (quadratic) and the constraints are linear, the necessary conditions lead to a system of linear equations, which is solved easily.

The SQP approach tries to exploit the aforementioned special features of the quadratic programming problems in order to solve the general nonlinear programming problem. At each iteration point $\mathbf{x}^{(k)}$, an appropriate quadratic programming problem is stated that is an approximation to the real problem. A sequential application of this technique leads from point $\mathbf{x}^{(k)}$ to point $\mathbf{x}^{(k+1)}$, until convergence to the optimum point $\mathbf{x}^*$. A complete presentation of the procedure and application examples appear in [Reklaitis et al. 1983, Rao 1996, Papalambros and Wilde 2000].

5.4 Decomposition

If an optimization problem is of separable form, i.e., if it can be written in the form

$$\min_{\mathbf{x}} f(\mathbf{x}) = \sum_{k=1}^{K} f_k(\mathbf{x}_k) \tag{5.31a}$$

subject to

$$\mathbf{h}_k(\mathbf{x}_k) = 0 \qquad k = 1, 2, \ldots, K \tag{5.31b}$$

$$\mathbf{g}_k(\mathbf{x}_k) \le 0 \qquad k = 1, 2, \ldots, K \tag{5.31c}$$

where the set **x** of the independent variables is partitioned into k disjoint sets,

$$\mathbf{x} = \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_K \tag{5.32}$$

then the problem can be decomposed into K separate subproblems:

$$\min_{\mathbf{x}_k} f_k(\mathbf{x}_k) \tag{5.33a}$$

subject to

$$\mathbf{h}_k(\mathbf{x}_k) = 0 \tag{5.33b}$$

$$\mathbf{g}_k(\mathbf{x}_k) \le 0 \tag{5.33c}$$

Each subproblem is solved independently from the other subproblems and the solution thus obtained is the solution of the initial problem too. Since each subproblem has a smaller number of independent variables and constraints than the whole problem, its solution is much easier; this is the main reason for applying decomposition.

The main application is the decomposition of a system into subsystems (or components), in which case f_k and $\mathbf{x}_k$ are the objective function and the set of the independent variables for the *k*th subsystem (or component). Another application of decomposition is in operation optimization over a number of independent time intervals (if it can be assumed that the operation in a time interval does not affect the operation in other time intervals).

5.5 Procedure for Solution of the Problem by a Mathematical Optimization Algorithm

Analytical application of the necessary and sufficient conditions is possible in rather simple optimization problems. For most of the optimization problems in energy systems, a numerical solution is necessary. Several general-purpose (i.e., not restricted to energy systems) algorithms have been developed, based on methods mentioned in Subsections 5.2 and 5.3, and related software is available. The most efficient and robust algorithms for nonlinear problems with many decision variables have proved to be those based on the generalized reduced gradient (GRG) method and on sequential quadratic programming (SQP). A few sources of optimization software are given in the Appendix.

The computer program, that the user has to develop for the solution of the optimization problem, consists of the following parts.

Main program: It reads the values of the parameters, the initial values of the independent variables (starting point) and the lower and upper bounds on the constraint functions. Then, it calls the optimization algorithm.

Simulation package (in the simplest case, a double precision function): For every set of values of the independent variables, it evaluates the dependent variables and the objective function. It is called by the optimization algorithm.

Constraints subroutine: It determines the values of the inequality constraint functions. It is called by the optimization algorithm. The equality constraint functions could be included in this subroutine, but it has been found more convenient and efficient to include these in the simulation package.

Optimization algorithm: Starting from the given initial point, it searches for the optimum. It prints intermediate and final results, messages regarding convergence, number of function evaluation, etc.

Nonlinear programming algorithms such as GRG and SQP cannot automatically locate the global optimum, if the objective function is multimodal. There are two approaches to search for the global optimum: (a) The user may solve the problem repeatedly starting from different points in the domain where $\mathbf{x}$ is defined. Of course, there is no guarantee that the global optimum is reached. (b) A coarse search of the domain is first conducted by, e.g., a genetic algorithm. Then, the points with the most promising values of the objective function are used as starting points with a nonlinear programming algorithm in order to determine the optimum point accurately. The second approach has a high probability for locating the global optimum.

5.6 Multilevel Optimization

The synthesis-design-operation optimization of complex systems under time-varying operating conditions involves a large number of variables and constraints. The optimization problem may become intractable even by the most capable software and hardware available. Multilevel optimization may help in these cases.

In multilevel optimization, the problem is reformulated as a set of subproblems and a coordination problem, which preserves the coupling among the subproblems. Multilevel optimization can be combined with decomposition either of the system into subsystems or of the whole period of operation into a series of time intervals or both.

As an example, let the synthesis-design-operation optimization of an energy system be considered. The overall objective function can be written (constraints are not written here, for brevity) as

$$\min_{\mathbf{x},\mathbf{z}} f(\mathbf{x}, \mathbf{z}) \tag{5.34}$$

where

- **x** set of independent variables for operation,
- **z** set of independent variables for synthesis and design (it specifies existence of components and the design characteristics of components and of the system as a whole).

It is also considered that the period of operation consists of K time intervals independent of each other, the set x can be partitioned into K disjoint sets, Eq. (5.32), and an objective function can be defined for each time interval

$$\min_{\mathbf{x}_k} \phi_k(\mathbf{x}_k) \tag{5.35}$$

The overall objective function f depends on ϕ_k's, without necessarily being a simple summation of these. Then, the optimization problem is reformulated as a two-level problem, as follows.

First-level problem

For a fixed set **z***,

Find $\mathbf{x}_k^*$ that minimizes $\phi_k(\mathbf{x}_k, \mathbf{z}^*)$, k = 1, 2, …, K.

Second-level problem

It is stated as follows:

Find a new **z*** which minimizes $f(\mathbf{x}^*, \mathbf{z})$ where **x*** is the optimal solution of the first-level problem. The procedure is repeated until convergence is achieved. The iterative steps are the following (letter A or B indicates the first or second level, respectively).

B1. Select an initial set of values $\mathbf{z}^o$ for **z**.

A. Solve the K first-level optimization problems. For the first problem (k=1):

A1. Select an initial set of values $\mathbf{x}_1^o$ for $\mathbf{x}_1$.

A2. Call the first-level optimization algorithm to solve the problem stated by Eq. (5.35) for k=1. The solution gives the optimum set $\mathbf{x}_1^*$.

Repeat steps A1 and A2 for k = 2, 3, …, K. Thus, the optimum vector $\mathbf{x}^*$ is obtained.

B2. Use the results of level A to evaluate the overall objective f, and check for convergence (i.e., whether the optimality criteria are satisfied). If convergence has not been reached, select a new set of **z** and go to step A1.

Steps B1 and B2 are in fact performed by the second-level optimization algorithm.

In practice, it has been often successful to use a genetic algorithm for level B and a nonlinear programming algorithm (e.g., GRG) for level A optimization.

5.7 Modular Simulation and Optimization

Decomposition as described in Subsection 5.5 may often be impractical in complex systems, primarily due to the fact that the sets $\mathbf{x}_k$ are not disjoint. The modular approach helps a lot in these cases.

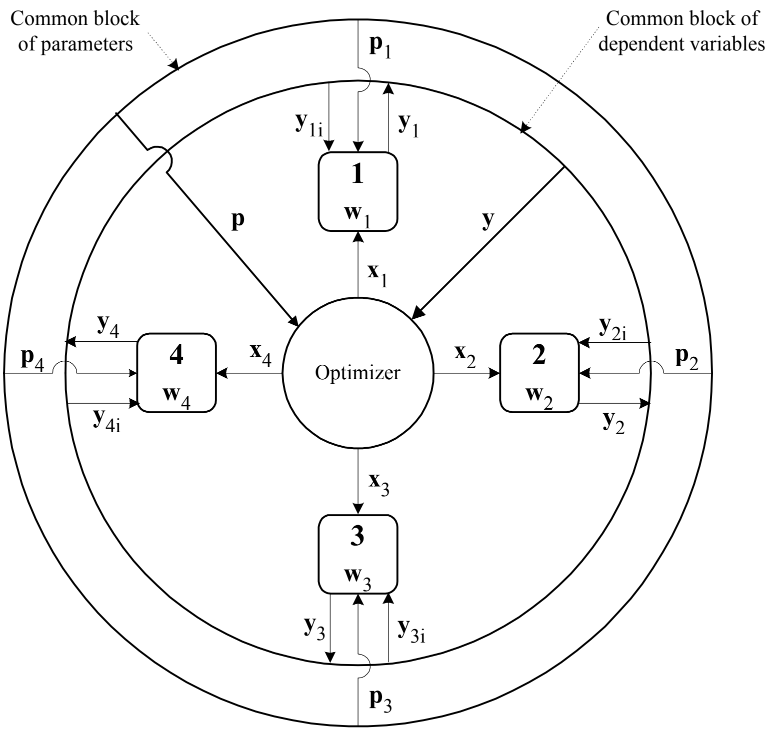

Fig. 5.8. Structure of the computer program for modular simulation and optimization. 1-4: Simulation and local optimization modules.

The system is considered as composed of modules. A module may consist of more than one component, if it facilitates the solution. A simulation model is developed for each module, which determines the dependent variables of the module as functions of the independent variables and the input dependent variables, i.e.,

$$\mathbf{y}_r = \mathbf{Y}(\mathbf{x}_r, \mathbf{y}_{ri}), \qquad \mathbf{w}_r = \mathbf{W}(\mathbf{x}_r, \mathbf{y}_{ri})$$

where

- $\mathbf{x}_r$ set of independent variables of module r (the sets $\mathbf{x}_r$ need not be disjoint),
- $\mathbf{y}_{ri}$ set of input dependent variables (coming from other modules),
- $\mathbf{y}_r$ set of output dependent variables of module r, i.e., of dependent variables which are used also by the simulation models of other modules or by the optimization algorithm,
- $\mathbf{w}_r$set of dependent variables appearing in the simulation model of module r only.

The structure of the computer program and the optimization procedure are explained by means of Fig. 5.8, as follows. The parts of the computer program described above are included in the optimizer (Fig. 5.8). In addition, the program contains the simulation subroutines. For every set of values **x**, given by the optimization algorithm, the simulation subroutines are called one after the other in such a way that iterations among modules are avoided or reduced to the minimum possible. The output dependent variables $\mathbf{y}_r$ are communicated to the simulation subroutines and the optimizer through common blocks. After a complete run of the simulation subroutines, the objective function is evaluated. The optimization algorithm updates the independent variables and the procedure is repeated until the convergence criteria are satisfied. If decomposition is applicable, then local optimization can be performed in one or more modules.

5.8 Parallel Processing

Optimization problems with many independent variables and detailed simulation models may take days to be solved by a computer, which is discouraging to the designer or operator of an energy system. These problems can be solved more efficiently (at a fraction of the initial time) by using parallel computers, i.e., multiple processing units combined in an organized way such that multiple independent computations for the same problem can be performed concurrently.

The modular approach and the decomposition are particularly suited for parallel processing: the simulation and/or optimization of modules or subsystems can be performed on parallel processors, while the coordinating optimization problem (optimizer in Fig. 5.8) can be solved by the main processor. Parallel processing can be used also with multilevel optimization. For the structure presented in Subsection 5.6, level A optimization subproblems can be solved on parallel processors, while level B optimization is performed on the main processor.

6. SPECIAL METHODS FOR OPTIMIZATION OF ENERGY SYSTEMS

The direct application of a mathematical programming method for the optimization of a complex energy system may often be inefficient or incapable of solving the problem. In order to overcome this difficulty, special methods have been (and continue being) developed. They proceed first with a proper analysis of the system (thermodynamic, economic, environmental, etc.) the results of which are used to direct the solution towards the optimum point. Along the way, a pure mathematical optimization method (algorithm) may be applied, if necessary, as described in Section 5. Representative special methods are described in brief in the following.

6.1 Methods for Optimization of Heat Exchanger Networks

The design of heat exchanger networks (HEN) is the most advanced area in synthesis optimization. This is due to the importance of minimizing energy costs and improving the energy recovery in chemical processes. The HEN synthesis problem can be stated as follows:

> *A set of hot process streams (HP) to be cooled, and a set of cold process streams (CP) to be heated are given. Each hot and cold process stream has a specified heat capacity flowrate while their inlet and outlet temperature can be specified exactly or given as inequalities. A set of hot utilities (HU) and a set of cold utilities (CU) along with their corresponding temperatures are also provided.*
> *Determine the heat exchanger network with the least total annualized cost.*

The solution of the optimization problem provides the

- hot and cold utilities required,
- stream matches and the number of heat exchangers,
- heat load of each heat exchanger,
- network configuration with flowrates and temperatures of all streams, and
- areas of heat exchangers.

Several methods have been developed since the 1960s for solving this problem. They can be classified in four main classes.

a. Heuristic methods

They attempt to synthesize very quickly one network using various heuristics (rules of thumb), which are the result of experience and of knowledge of various processes. The networks they lead to cannot be guaranteed to be the best, but experience has shown that they are close to optimum.

b. Search methods

When the number of hot and cold streams is increased, heuristic methods may not be very successful. A different approach is followed. First, a systematic way is developed for generating all possible heat-exchange networks for the given hot and cold streams. Then, a strategy is developed that evaluates a few networks to establish the direction for locating the optimum one. The tree-branching method, evolutionary synthesis, and the forward-branching and bounding are among the methods in this class.

However, the number of matches between the hot and cold streams grows so rapidly with the number of streams, that it is practically impossible to identify all possible matches, when a large number of streams is involved. Therefore, more efficient methods are needed.

c. Pinch method

The key concept of this method is the pinch point, i.e., the point (temperature) at which the temperature versus heat flowrate composite curve of the hot streams most closely approaches the temperature versus heat flowrate composite curve of the cold streams. If heat exchange takes place between streams above or below the pinch, but not along the pinch, then the requirements for hot and cold utilities are minimum. Thus, the best possible energy performance (target of minimum utility needs) is first predicted, before design. Next, a design, which satisfies this energy target is synthesized. Finally, the network is evolved towards minimum total cost. The method has been applied in hundreds of process industries resulting in energy savings typically in the range of 20-50%. It is described in detail in the publications by Linnhoff and his coworkers (representative publications are given in the bibliography). An instructive presentation with application examples appears also in the book by Bejan et al. (1996). The method has been further developed for optimization of utility systems, combined heat and power plants and heat pumps.

d. Mathematical programming methods

It can be argued that the decomposition of the HEN optimization problem into subtasks (minimization of utility needs, minimization of total cost) and the sequential solution (first, identification of the minimum utility design and, next, minimization of cost) may not lead to the real optimum (minimum cost) design.

In order to avoid these limitations, researchers in the late 1980s and early 1990s focused on simultaneous optimization approaches that attempt to treat the HEN synthesis problem as a single-task problem. Recent advances in theoretical and algorithmic aspects of optimization provide the tools needed for such a purpose. A superstructure is usually considered, and the optimal design is reached by applying a mixed integer nonlinear programming (MINLP) algorithm. This approach is presented in the book by Floudas (1995). Attempts have also been made to apply simulated annealing instead of MINLP algorithms.

e. Artificial Intelligence methods

It is a combination of the Heuristic, Pinch and Search methods. First, a suitable solution tree is developed, consisting not of all heat-exchange networks that can be constructed with the given streams mathematically, but only of those that abide by a set of physical and engineering rules. This tree by itself would already be strongly pruned. During its construction, though, AI methods are employed to further prune it by imposing formal constraints corresponding to "good" design practices, to the dictates of the Pinch method, and to proper Second Law considerations (basically, minimization of exergy losses). Cost considerations may be also included. The resulting set of solutions is an extremely slim tree, often consisting of only very few configurations among which the designer has then the choice. These methods have been proven to consistently give at least the same results of the other methods, with a much lesser computational effort on the part of the user. They are, though, as all Expert Systems, only as good as the Knowledge that has been formalized in their Knowledge Base [Sciubba and Melli 1998, Maiorano et al. 2002].

6.2 The First Thermoeconomic Optimization Method

Thermoeconomics appeared in the 1960s as a technique, which combines thermodynamic and economic analysis for the evaluation, improvement and optimization of thermal systems [Tribus and Evans 1962, Evans et al. 1966]. Economic considerations require a proper balance between an appropriate thermodynamic measure and capital expenditure, in order to achieve a minimum product cost. Introducing dissipation (exergy destruction) as a unified extensive measure, thermoeconomics considers the complex system as made up of a number of dissipative zones, for each of which the relative economic value of dissipation is estimated. A local balance between capital expenditure and dissipation is then made in each zone.

Two basic concepts are introduced: the concept of *exergy* and the concept of *internal economy*. Exergy provides a common basis for evaluation and comparison of processes, and a consistent way of evaluating dissipations. On the other hand, a structure of internal unit costs representing a fictitious internal economy is introduced to provide convenience in evaluating the overall relative economic values of local dissipations.

The balance between thermodynamic measures and capital expenditures is an economic feature, which applies to the complex plant as a whole and to each of its components individually. This feature makes it feasible to attain, in most cases, physical decomposition on the basis of a unified thermodynamic measure without violating the mathematical disciplines of optimization.

The method is presented in [El–Sayed and Aplenc 1970, El-Sayed and Evans 1970, El-Sayed and Tribus 1981].

6.3 The Functional Approach

The functional approach is an offspring of the thermoeconomic method described in the preceding subsection. It appeared initially under the name Thermoeconomic Functional Analysis (TFA), while further developments bear the names Intelligent Functional Approach (IFA) and Engineering Functional Analysis (EFA) [Frangopoulos 1983, 1987, 1990, von Spakovsky and Evans 1993, Evans and von Spakovsky 1993]. The general formulation of the method as well as the special forms of decomposition are described in brief in the following. Further developments of decomposition can be found in [Munoz and von Spakovsky 2001].

6.3.1 Concepts and definitions

A thermal power plant or a chemical plant can be considered as a “system”, i.e. “a set of interrelated units, of which no unit is unrelated to any other unit,” where “unit” is “a piece or complex of apparatus serving to perform one particular function” (in this case, apparatus is the system itself). A system can be viewed also as a “time-varying configuration of men, hardware, and operating procedures grouped together for the purpose of accomplishing a useful function(s)”.

The word “function” here has the following meaning: “Function, referable to anything living, material or constructed, implies a definite end or purpose that the one in question serves or a particular kind of work it is intended to perform”. Thus, “Functional Analysis” does not imply that particular branch of mathematics, but it is the formal, documented determination of the functions of the system as a whole and of each unit individually.

It is appropriate here to distinguish between a unit and a component. For example, a cooling tower or a cooling water circulating pump are components in themselves. However, they may not be considered as separate units but, combined with the condenser, they may form only one unit with one function. The number of units in a plant is not unique; it depends on the available information and the requested results. The designer will stay at a resolution level, which is satisfactory for his objectives. He/she may go to a resolution level higher (more units), or lower (fewer units), if this serves better his/her objectives.

6.3.2 The Functional diagram of a system

The picture of a system in this analysis will be composed primarily of the units represented by small geometrical figures, and lines connecting the units, which represent the relations between units or between the system and the environment. Since the relations are established by distribution of the unit functions, (i.e. “services” or “products”), this picture will be called the “Functional Diagram” of the system. Which direction a function (“service”) goes will be indicated by arrows on the lines.

In the functional diagram, each unit is shown as in Fig. 6.1.

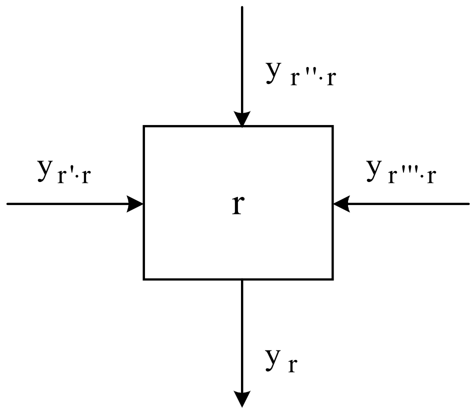

Fig. 6.1. Unit.

where

r	the r_{th} unit of the system ($r = 1, 2, ..., \sigma$),
y_r	the product, i.e. the appropriate quantitative description of the function of unit r,
$y_{r'\cdot r}, y_{r''\cdot r}, \ldots$	functions used by unit r, which come from other units of the system or the environment; in particular, the environment is represented by r = 0.

It should be emphasized that a $y_{r'\cdot r}$ (a line with an arrow pointing towards a unit) does not necessarily represent a stream (of mass, energy, etc.) entering the unit. For example, exhaust gases of a boiler form a stream exiting the boiler, but the service of getting rid of exhaust gases is provided to the boiler by another unit. Similarly, if the boiler is to be penalized for environmental pollution, then the corresponding expenditure will depend on an appropriate measure of pollution, $y_{0k\cdot r}$, which is depicted as an arrow pointing toward the unit (the subscript 0k·r denotes the k_{th} function provided by the environment to the unit r).

There are cases where the functions of two or more units merge, and other cases where the function of a unit is distributed to more than one unit. They are represented by “junctions” and “branching points”, respectively (Figs. 6.2 and 6.3).

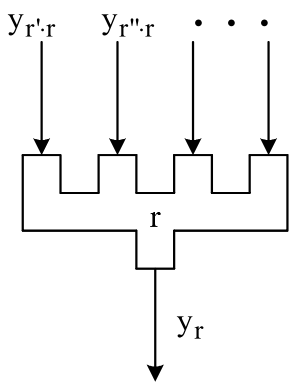

Figure 6.2. Junction.

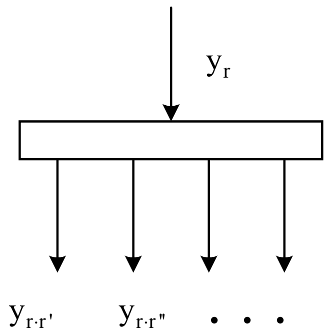

Figure 6.3. Branching point.

A junction or a branching point is considered a fictitious unit, except if it corresponds to a real component of the plant. The following relationships are applicable.

For a junction : $$\sum_{r'=0}^{R} y_{r'\cdot r} = y_r \ , \qquad r = \sigma+1, \sigma+2, ..., R \qquad (6.1)$$

where R is the number of units and junctions.

For a branching point : $$y_r = \sum_{r'=0}^{R} y_{r\cdot r'} \ , \qquad r = 1, 2,\ldots, R \qquad (6.2)$$

Using the rules established above, the functional diagram of a system can be drawn. The procedure will be demonstrated in another section by an example.

The functional analysis consists of two main actions:

1. Identification of the functions of the system as a whole and of each unit individually.
2. Drawing the functional diagram of the system.

Additional actions are required when optimization is required, as it will be explained below.

6.3.3 Thermoeconomic Functional Analysis

The assessment of the performance of an energy system has to be based on a consistent consideration of benefits and hazards associated with the construction and operation of the system. For this purpose, the benefits and hazards have to be properly quantified and assigned economic values. Even though this may be an arduous task, it is considered here that it is completed to the maximum possible. An economic function, which fulfills these requirements, is the total cost for construction and operation of the system (life cycle cost), with benefits (e.g. revenue from products) taken into consideration as negative costs:

$$F = \sum_r Z_r + \sum_r \sum_k \Gamma_{0k\cdot r} - \sum_r \Gamma_{r\cdot 0} \tag{6.3}$$

On the right hand side of Eq. (6.3), the first term represents the capital cost of the system including fixed charges, maintenance, decommissioning, etc. The second term represents costs of resources and services supplied to the system by the environment, as well as penalties imposed on the system for hazards it causes to the environment (e.g. pollution). The third term represents revenue from products or services the system provides to the environment.

The terms in Eq. (6.3) are derived by an integration over time. If a steady-state operation can be assumed, at least in certain time intervals, cost rates can be used

$$\dot{F} = \sum_r \dot{Z}_r + \sum_r \sum_k \dot{\Gamma}_{0k\cdot r} - \sum_r \dot{\Gamma}_{r\cdot 0} \tag{6.4}$$

which very often facilitate the analysis.

It is important to point out that all the terms in Eqs. (6.3) and (6.4) can be evaluated either in monetary units or in physical units (e.g., energy, exergy). The latter case is known as the "physical economics" approach.

In the functional analysis, all costs are expressed as mathematical functions of certain decision variables characterizing the construction and operation of the units, and of the quantities purchased or sold:

$$\dot{Z}_r = Z_r(\mathbf{x}_r, y_r) \equiv Z_r \tag{6.5a}$$

$$\dot{\Gamma}_{0k\cdot r} = \Gamma_{0k\cdot r}(y_{0k\cdot r}) \equiv \Gamma_{0k\cdot r} \tag{6.5b}$$

$$\dot{\Gamma}_{r\cdot 0} = \Gamma_{r\cdot 0}(y_{r\cdot 0}) \equiv \Gamma_{r\cdot 0} \tag{6.5c}$$

$$\dot{F} = F(\mathbf{x}, \mathbf{y}) = F \tag{6.5d}$$

Both sides of Eqs. (6.5) are expressions for cost rate, but the left hand side (e.g. $\dot{Z}_r$) symbolizes the cost rate quantity itself, while the right hand side (e.g. Z_r) symbolizes the mathematical functional operation, which generates its numerical value. Then, Eq. (6.4) can be written:

$$F(\mathbf{x}, \mathbf{y}) = \sum_r Z_r(\mathbf{x}, y_r) + \sum_r \sum_k \Gamma_{0k\cdot r}(y_{0k\cdot r}) - \sum_r \Gamma_{r\cdot 0}(y_{r\cdot 0}) \tag{6.6}$$

By the technical analysis of the system, mathematical functions are derived, which give the input to a unit as a function of the unique product (function) of the unit and its decision variables:

$$y_{r\cdot r'} = Y_{r\cdot r'}(\mathbf{x}_{r'}, y_{r'}) \equiv Y_{r\cdot r'}, \qquad r' = 1, 2, \ldots, R \qquad r = 0, 1, 2, \ldots, R \tag{6.7}$$

Interconnections between units or between a unit and the environment are revealed also by equations of the form

$$y_r = \sum_{r'=0}^{R} y_{r \cdot r'}, \qquad r = 1, 2, \ldots, R \tag{6.8}$$

If any product of the system is quantitatively fixed, then for this product it is

$$y_{r \cdot 0} = \hat{y}_{r \cdot 0} \tag{6.9}$$

where $\hat{y}_{r \cdot 0}$ is the fixed (known) quantity of the particular product (e.g. electric power $\dot{W}$, thermal power $\dot{Q}$, etc.).

Equations (6.3)-(6.9) are the fundamental equations, which are used either for analysis based on average unit costs of the products-functions or for optimization, in which case marginal costs are derived. For analysis, it is useful to write a cost balance for each unit, assuming a break-even operation, i.e., no profit-no loss:

$$C_r \equiv Z_r + \sum_{r'=0}^{R} c_{r'} \, y_{r' \cdot r} = c_r \, y_r, \quad r = 1, 2, \ldots, R \tag{6.10}$$

The system of Eqs. (6.10) can be solved for the average unit product costs c_r. In writing Eq. (6.10), it is taken into consideration that a branching point does not cause any change in the unit cost of the function (product) it distributes. Also, it is clarified that a junction does not have capital cost, i.e., $Z_r = 0$, $r = \sigma+1, \sigma+2, \ldots, R$.

6.3.4 Functional Optimization

Minimization of the total cost, as it is given by Eqs. (6.3), (6.4) or (6.6), is selected as the optimization objective. Let us continue with Eq. (6.6), which is written as an objective function:

$$\min F = \sum_r Z_r(\mathbf{x}, y_r) + \sum_r \sum_k \Gamma_{0k \cdot r}(y_{0k \cdot r}) - \sum_r \Gamma_{r \cdot 0}(y_{r \cdot 0}) \tag{6.11}$$

Equations (6.7) and (6.8) are the equality constraints. The method of Lagrange multipliers is used for the solution of the optimization problem, for reasons that will become clear in the following. The Lagrangian is written:

$$L = \sum_r Z_r + \sum_r \sum_k \Gamma_{0k \cdot r} - \sum_r \Gamma_{r \cdot 0} + \sum_{r'} \sum_r \lambda_{r \cdot r'}(Y_{r \cdot r'} - y_{r \cdot r'}) + \sum_r \lambda_r (\sum_{r'} y_{r \cdot r'} - y_r) \tag{6.12}$$

The first order necessary conditions for an extremum are:

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \mathbf{y}, \lambda) = 0 \tag{6.13a}$$

$$\nabla_{\mathbf{y}} L(\mathbf{x}, \mathbf{y}, \lambda) = 0 \tag{6.13b}$$

$$\nabla_{\lambda} L(\mathbf{x}, \mathbf{y}, \lambda) = 0 \tag{6.13c}$$

In particular, the conditions

$$\frac{\partial L}{\partial y_{r \cdot r'}} = 0$$

which are part of Eqs. (6.13b), applied on Eq. (6.12) give

$$\lambda_{r \cdot r'} = \lambda_r \tag{6.14}$$

i.e. the Lagrange multiplier $\lambda_{r \cdot r'}$ associated with an input $y_{r \cdot r'}$ is equal to the Lagrange multiplier λ_r associated with that output y_r, which supplies the $y_{r \cdot r'}$. Then, the Lagrangian can be written in the convenient form

$$L = \sum_r (\Gamma_r - \lambda_r y_r) + \sum_r \sum_k (\Gamma_{0k \cdot r} - \lambda_{0k \cdot r} y_{0k \cdot r}) - \sum_r (\Gamma_{r \cdot 0} - \lambda_{r \cdot 0} y_{r \cdot 0}) \tag{6.15}$$

where

$$\Gamma_r = Z_r + \sum_{r'=0}^{R} \lambda_{r' \cdot r} Y_{r' \cdot r}, \quad r = 1, 2, \ldots, R \tag{6.16}$$

The conditions (6.13) applied on Eq. (6.15) give the equations

$$\nabla_{\mathbf{x}} \sum_r \Gamma_r = 0 \tag{6.17a}$$

$$\lambda_r = \frac{\partial \Gamma_r}{\partial y_r} \tag{6.17b}$$

$$\lambda_{0k \cdot r} = \frac{\partial \Gamma_{0k \cdot r}}{\partial y_{0k \cdot r}} \tag{6.17c}$$

$$\lambda_{r \cdot 0} = \frac{\partial \Gamma_{r \cdot 0}}{\partial y_{r \cdot 0}} \tag{6.17d}$$

The solution of the system of Eqs. (6.17) gives the optimum values of the unknown **x**, **y**, **λ**. It is noted that, if a product is not quantitatively fixed (predetermined), the solution of the problem gives also the optimum production rate. For a quantitatively fixed product, there is no need to know the function $\Gamma_{r \cdot 0}(y_{r \cdot 0})$, and the corresponding term does not appear in Eq. (6.15).

Equations (6.16) and (6.17) lead to an interpretation of the Lagrange multipliers as economic indicators: each λ can be viewed as the marginal price (cost or revenue) of the corresponding function (product) y. Consequently, the Lagrange multipliers reveal one more aspect of the internal economy of the system. This is one of the main reasons for selecting the method of Lagrange multipliers in order to solve the optimization problem. One more reason is that the method leads readily to decomposition, which facilitates the solution of large optimization problems.

6.3.5 Complete functional decomposition

The conditions for decomposition have been stated in Subsection 5.4. It is noted that the objective function and the constraints in the functional approach, Eqs. (6.11), (6.7) and (6.8), are of separable form. In the general formulation of the functional optimization, the sets of decision variables $\mathbf{x}_r$ are not required to be disjoint. If this requirement is satisfied, then decomposition is applicable and the subsystems correspond to the units and junctions of the system, i.e.,

$$q = R \tag{6.18}$$

Such a case is called *complete functional decomposition*. The sub-problem of each unit r is described by the system of equations

$$\nabla_{\mathbf{x}_r} \Gamma_r = 0 \tag{6.19a}$$

$$Y_{r \cdot r'}(\mathbf{x}_{r'}, y_{r'}) - y_{r \cdot r'} = 0 \tag{6.19b}$$

$$\lambda_r = \frac{\partial \Gamma_r}{\partial y_r} \tag{6.19c}$$

Equations (6.19) show that, under conditions of decomposition, each unit may be considered as optimized for its own objective function:

$$\min_{\mathbf{x}_r} \Gamma_r = Z_r + \sum_{r'=0}^{R} \lambda_{r' \cdot r} \ Y_{r' \cdot r} \tag{6.20a}$$

subject to the constraints

$$y_{r' \cdot r} = Y_{r' \cdot r}(\mathbf{x}_r, y_r) \tag{6.20b}$$

Each $\lambda_{r' \cdot r}$ is the marginal cost of the corresponding $y_{r' \cdot r}$. Hence, the objective (6.20a) may be interpreted as the minimization of the total cost of owning and operating the unit r, although for such an interpretation to be precise, each $\lambda_{r' \cdot r}$ should be a unit cost independent of the magnitude of $y_{r' \cdot r}$, which is valid in case of cost functions linear with respect to $y_{r' \cdot r}$.

The solution of the system of Eqs. (6.19) gives the optimum values of the independent variables and the Lagrange multipliers.

6.3.6 Partial functional decomposition

If the sets $\mathbf{x}_r$ are not disjoint, but it is possible to formulate larger sets $\mathbf{x}_v$, $(v = 1, 2, ..., q < R)$, which are disjoint, then decomposition is applicable again, although of a lower level. Such a case is called *partial functional decomposition*. All the decision variables that belong to a set $\mathbf{x}_r$, must belong to the same set $\mathbf{x}_v$. This requirement places a restriction (and at the same time suggests) how the R units and junctions of the system can be grouped into q subsystems. The optimum values of the decision variables of each subsystem must satisfy the equation

$$\nabla_{\mathbf{x}_\nu} \Gamma_\nu = 0 \tag{6.21}$$

where

$$\Gamma_\nu = \sum_r \Gamma_r \tag{6.22}$$

The summation in Eq. (6.22) is considered over those units and junctions, which belong to the subsystem ν. Equations (6.19b) and (6.19c) are valid. The solution of the system of Eqs. (6.21), (6.19b,c) gives the optimum values of the independent variables and the Lagrange multipliers.

6.4 Artificial Intelligence Techniques

In the optimization methods mentioned in the preceding sections, the problem is well defined with respect to both the data and the goals (objectives), and the solution is obtained by deterministic as well as heuristic methods and algorithms. This approach produces satisfactory results in many cases, and it has been and still is of invaluable practical usefulness. However, real-world problems are often not "textbook" problems: though the goals may be well defined, data are often incomplete and expressed in qualitative instead of quantitative form; furthermore, the constraints are weak or even vague. Nevertheless, these cases must be handled by the engineers. To help the engineer in this task, new procedures have been developed under the general denomination of "expert systems" or "artificial intelligence". The field is developing rapidly. Related information can be found in [Sciubba and Melli, 1998].

7. INTRODUCTION OF ENVIRONMENTAL AND SUSTAINABILITY CONSIDERATIONS IN THE OPTIMIZATION OF ENERGY SYSTEMS

7.1 Principal Concerns

During the 1970s and 1980s, one of the main concerns about the design and operation of energy systems has been the depletion of energy (exergy) resources. *Thermoeconomics, exergoeconomics,* and other similar terms were used to imply the combined thermodynamic and economic analysis of energy systems, which helps in increasing the efficiency of a plant without jeopardizing its economic viability. Of course, increasing the efficiency may result in a decrease of adverse environmental effects, but this was not the principal driving force behind the whole activity.

In the 1990s, the effort to improve efficiency and develop alternative energy technologies continued. However, since much of the blame for exploitation of (not only energy) resources and degradation of the environment goes to the construction and operation of energy systems, the focus of research and development of these systems has turned to the protection of the environment. Methods of analysis and optimization have been further developed to take into consideration not only energy use (exergy consumption) and financial resources expended (economics), but also the scarcity of physical resources used as well as any pollution and degradation of the environment resulting from an energy system. Furthermore, these effects are accounted for the entire life cycle of the system, starting with initial conception and ending with decommissioning of the plant and recycling of materials. The term *environomics* appeared in the literature to express the fact that environmental consequences are taken quantitatively into consideration in the analysis [Frangopoulos 1991].

In order to introduce sustainability into the analysis of energy systems, three aspects have to be considered:

a. scarcity of natural resources,
b. degradation of the natural environment, and
c. social implications of the energy system, both positive (e.g. job creation, general welfare) and negative (effects on human health).

Two approaches have appeared, which attempt to take the aforementioned aspects quantitatively into consideration for the analysis and optimization of energy systems: (a) sustainability indicators, and (b) total cost function. Information about the first one can be found in [Afgan and Carvalho, 2000]. The second one is described in brief in the following. It is true that these methods are not fully developed yet, and the data required for a complete analysis are still not all available. Consequently, a considerable effort is required at an international level in order for sustainability considerations to be fully integrated in energy systems analysis and design.

7.2 The New Objective

7.2.1 Total cost function

In this approach, a total cost function is defined, which includes the extraction of raw materials, the manufacture of equipment, the construction of the plant, operating expenses, cost of resources, environmental (including social) cost, and expenses for dismantling used-up equipment and recycling of the material. An important term in this cost function is the internalized external environmental cost. Equation (6.11) is now written:

$$\min \mathrm{F} = \sum_{r} Z_r + \sum_{r}\sum_{k} \Gamma_{0k\cdot r} + \sum_{e} \Gamma_e - \sum_{r} \Gamma_{r\cdot 0} \tag{7.1}$$

where Γ_e is the *e*th environmental and social cost due to construction and operation of the system. The first term on the right hand side of Eq. (7.1) includes, among other components, the cost of equipment installed in the plant for pollution abatement.

Another way of writing the total cost is:

$$\begin{aligned} \text{Total cost} = {} & \text{Internal general cost} \\ & + \text{Internal environmental cost} \\ & + \text{External environmental cost} \end{aligned} \tag{7.2}$$

Internal general cost is the cost of energy supply, excluding environmental protection or safety measures. Costs of an industrial activity related to environmental protection (e.g. costs of equipment to clean the exhaust gases before they are released into the atmosphere) are called *internal environmental costs*. Other environmental costs related to the activity are born by the society, rather than paid for, e.g., in electricity bills. The unpaid costs are called *external environmental costs*. It is worth noting that some of the people who bear these costs may not benefit from the particular industrial activity, e.g. in transboundary pollution. In writing Eq. (7.1) or (7.2) attempt is made to internalize the external environmental costs.

7.2.2 Cost of resources

Regarding the scarcity of resources, one might say that scarcity is taken into consideration by their price: more scarce resources should have a higher price. However, this price reflects short-term considerations only. A quantity of raw material extracted today has two consequences: (a) it will not be available for future generations, and (b) it will cause future generations to spend more energy for extracting the remaining quantities of the same material. Even though current market prices, whether artificial or real, reflect the costs of extraction and present or near-future term supply and demand, they do not, in general, account for long-term local or global scarcity or the ensuing difficulties and costs of extraction that such scarcity may cause. A method to correct (to a certain extent) this deficiency is to introduce properly defined *scarcity factors* into the analysis.

The general cost function of a resource, Eq. (6.5b), can take any form; an example might be the following:

$$\Gamma_{0k\cdot r} = f_{p0k\cdot r} f_{s0k\cdot r} c_{0k\cdot r} y_{0k\cdot r} \tag{7.3}$$

where

$c_{0k\cdot r}$ unit cost of resource $0k\cdot r$ (e.g. market price),

$f_{p0k\cdot r}$ pollution penalty factor for resource $0k\cdot r$ (it accounts for extraction, processing and transportation of the resource; pollutants emitted while the resource is used, e.g. during combustion of a fuel, are treated in separate),

$f_{s0k\cdot r}$ scarcity factor for resource $0k\cdot r$; it accounts for difficulties in extracting a particular resource and for the local and/or future scarcity of the resource.

7.2.3 Pollution measures and costs

Each pollutant emitted to the environment causes a cost to the society, which can be expressed as a general function:

$$\Gamma_e = \Gamma_e(p_e) \tag{7.4}$$

where p_e is an appropriate measure of pollution. It is very difficult to derive analytic expressions for this function. At least a simple expression such as the following can be used:

$$\Gamma_e = f_{pe} c_e p_e \tag{7.5}$$

where

c_e unit environmental and social cost due to the pollutant e,
f_{pe} pollution penalty factor for the pollutant e.

The pollution measure, p_e, can be expressed in various forms: it can be the quantity of the pollutant (e.g. kg of CO_2), the exergy content of the pollutant, the entropy increase of the environment due to the pollutant, etc.

Regarding the environmental and social cost due to pollution, three approaches have been identified in the literature, which attempt to estimate it:

(i) *Indirect methods*: they aim at measuring the value of goods not traded in formal markets, such as life, scenic and recreational goods, which are affected by the pollution.
(ii) *Direct methods (damage cost)*: they are used to measure goods for which economic costs can be readily assessed, such as the value of agricultural products, or the cost of repairing damaged goods.
(iii) *Proxy methods (avoidable cost)*: they are used to measure the costs of avoiding the initiating insult, rather than the cost of damage created by the insult.

Many studies have been and continue being performed in the attempt to estimate the environmental costs. Lack of sufficient data, limited epistemological position and other difficulties may cause an uncertainty in the numerical results obtained. However, an attempt to derive reasonable figures and take these into consideration in the analysis and optimization makes far more sense than to ignore external effects of energy systems.

More information about the pollution measures, unit environmental and social costs due to the pollution, pollution factors and scarcity factors can be found in the literature [EC 1999, Gaivao and Jaumotte 1985, Hohmeyer 1988, Ottinger R. et al. 1990, Frangopoulos 1992, Frangopoulos and von Spakovsky 1993, Frangopoulos and Caralis 1997].

8. SENSITIVITY ANALYSIS

8.1 Sensitivity Analysis with respect to the Parameters

It is also called simply *sensitivity analysis* or *parametric analysis*.

The optimization problem is initially solved for a certain set of values for the parameters. However, the values of many parameters (e.g. costs) are not known with absolute accuracy, but they are derived as a result of statistical estimates or predictions for the future. Therefore, it is necessary to perform a sensitivity analysis, i.e. to study the effect that a change in the values of important parameters may have on the optimal solution. This effect can be revealed by at least three methods, as explained below.

A. Preparation of graphs

The optimization problem is solved for several values of a single parameter, while the values of the other parameters are kept constant. Then, graphs are drawn, which show the optimal values of the independent variables and of the objective function as functions of the particular parameter.

B. Evaluation of the uncertainty of the objective function

If p_j, j = 1, 2, …. are the parameters of the optimization problem, one or more of the following quantities are evaluated.

Uncertainty of the objective function due to the uncertainty of a parameter:

$$\Delta F = \frac{\partial F}{\partial p_j} \Delta p_j \tag{8.1}$$

Maximum uncertainty of the objective function due to the uncertainties of a set of parameters:

$$\Delta F_{max} = \sum_j \left| \frac{\partial F}{\partial p_j} \right| \Delta p_j \tag{8.2}$$

The most probable uncertainty of the objective function due to the uncertainties of a set of parameters:

$$\Delta F_{prob} = \sqrt{\sum_j \left[\frac{\partial F}{\partial p_j} \Delta p_j \right]^2} \tag{8.3}$$

C. Evaluation of certain Lagrange multipliers

If the constraints of the optimization problem are written in the form

$$h_j(\mathbf{x}) = p_j \tag{8.4a}$$

$$g_k(\mathbf{x}) \le p_k \tag{8.4b}$$

where p_j, p_k are parameters, then the Lagrangian is written

$$L = F(\mathbf{x}) + \sum_j \lambda_j \left[p_j - h_j(\mathbf{x}) \right] + \sum_k \mu_k \left[p_k - g_k(\mathbf{x}) \right] \tag{8.5}$$

It is

$$\lambda_j = \frac{\partial L}{\partial p_j}, \qquad \mu_k = \frac{\partial L}{\partial p_k} \tag{8.6}$$

At the optimum point, for the p_j's and those of the p_k's for which Eq. (8.4b) is valid as equality, it is

$$\frac{\partial L}{\partial p_j} = \frac{\partial F}{\partial p_j}, \qquad \frac{\partial L}{\partial p_k} = \frac{\partial F}{\partial p_k} \tag{8.7}$$

Equations (8.6) and (8.7) result in

$$\lambda_j = \frac{\partial F}{\partial p_j}, \qquad \mu_k = \frac{\partial F}{\partial p_k} \tag{8.8}$$

Consequently in this case, the uncertainty of the objective function is determined by means of the Lagrange multipliers.

If the sensitivity analysis reveals that the optimal solution is very sensitive with respect to a parameter, then one or more of the following actions may be necessary:

- attempt for a more accurate estimation of the parameter (decrease of the uncertainty of the parameter),
- modifications in the design of the system with the scope of reducing the uncertainty,
- changes in decisions regarding the use of (physical and economic) resources for the construction and operation of the system.

Since these actions may be of crucial importance for the implementation of a project, a careful sensitivity analysis may prove more useful than the solution of the optimization problem itself.

8.2 Sensitivity Analysis of the Objective Function with respect to the Independent Variables

There are cases where the optimum value of an independent variable cannot be selected in practice. For example, pipes are available at standard sizes. If the diameter of a pipe is an independent variable and the available optimization algorithm treats it as a continuous variable (not a discrete one), then the optimum value of the diameter may not be one of the standard sizes. Consequently in practice the diameter will not be equal to the optimum one. In such cases, it is useful to study the effect of a deviation from the optimum value of an independent variable to the value of the objective function.

The sensitivity of the optimum solution with respect to the independent variable x_i is revealed by the values of the following derivatives at the optimum point:

$$\left.\frac{\partial f(\mathbf{x})}{\partial x_i}\right|_{\mathbf{x}^*} \qquad \left.\frac{\partial x_j}{\partial x_i}\right|_{\mathbf{x}^*}, \qquad j \neq i$$

or with the differences

$$\left.\frac{\Delta f(\mathbf{x})}{\Delta x_i}\right|_{\mathbf{x}^*} \qquad \left.\frac{\Delta x_j}{\Delta x_i}\right|_{\mathbf{x}^*}$$

Note: The term “sensitivity analysis” will imply the sensitivity analysis with respect to the parameters, except if it is specified differently.

Further details on sensitivity analysis are given in the literature [e.g.. Rao 1996, Papalambros and Wilde 2000].

9. NUMERICAL EXAMPLES

Three examples of system optimization are given in this section. Additional examples can be found in several publications [e.g. Benini et al. 2001, Frangopoulos 1990, Frangopoulos and Dimopoulos 2001, Manolas et al. 1997, Munoz and von Spakovsky 2001, Maiorano et al. 2002].

9.1 Thermoeconomic Operation Optimization of a System[1]

Nomenclature for the particular example

$\dot{C}_{ar}$	capital cost rate of the subsystem r
$\dot{C}_{mr}$	maintenance cost rate of the subsystem r
$\dot{C}_{mpr}$	maintenance and personnel cost rate of the subsystem r
$\dot{C}_{pr}$	personnel cost rate of the subsystem r
c_{chf}	unit cost of chemicals for treating the total feed water
c_{cw}	unit cost of cooling water
c_{c1}	unit cost of treated condensate
c_D	unit cost of Diesel oil
c_{el}	unit cost of electricity purchased from the utility grid
c_{HG}	unit cost of high-pressure fuel gas
c_{LF}	unit cost of fuel oil
c_{LG}	unit cost of low-pressure fuel gas
c_{mpr}	unit cost for maintenance and personnel of subsystem r
c_{PR}	unit cost of propane
c_{w1}	unit cost of treated supplementary feed water
f, F	objective function
$\dot{m}_D$	mass flow rate (consumption) of Diesel oil
$\dot{m}_e$	mass flow rate of extracted steam from the steam turbine
$\dot{m}_{HG}$	mass flow rate (consumption) of high-pressure fuel gas
$\dot{m}_{LF}$	mass flow rate (consumption) of fuel oil
$\dot{m}_{LG}$	mass flow rate (consumption) of low-pressure fuel gas
$\dot{m}_{PR}$	mass flow rate (consumption) of propane
$\dot{m}_{sB}$	mass flow rate of steam produced by the fuel oil boilers
p_{el}	unit price of electricity sold to the utility grid
r	the *r*th subsystem
t	time
$\dot{V}_{cw}$	volumetric flow rate of cooling water through the condenser
$\dot{V}_{c1}$	volumetric flow rate of treated condensate
$\dot{V}_{w1}$	volumetric flow rate of treated supplementary feed water (make-up)

[1] Source: [Frangopoulos et al. 1996].

$\dot{V}_{w3}$ volumetric flow rate of the total feed water

$\dot{W}_A$ electric power for the auxiliary equipment of the system

$\dot{W}_b$ electric power purchased from the utility grid

$\dot{W}_{G1}$ electric power of gas-turbine generator No. 1

$\dot{W}_{G2}$ electric power of gas-turbine generator No. 2

$\dot{W}_{SG}$ electric power of steam-turbine generator

$\dot{W}_s$ electric power sold to the utility grid

x set of independent variables

9.1.1 Description of the system

A combined cycle cogeneration system (Fig. 9.1.1) covers the needs of a refinery in electricity and steam at four grades (Table 9.1.1). Interconnection with the utility grid allows for purchasing extra electricity, if needed, and selling excess electricity, if it is available and economical.

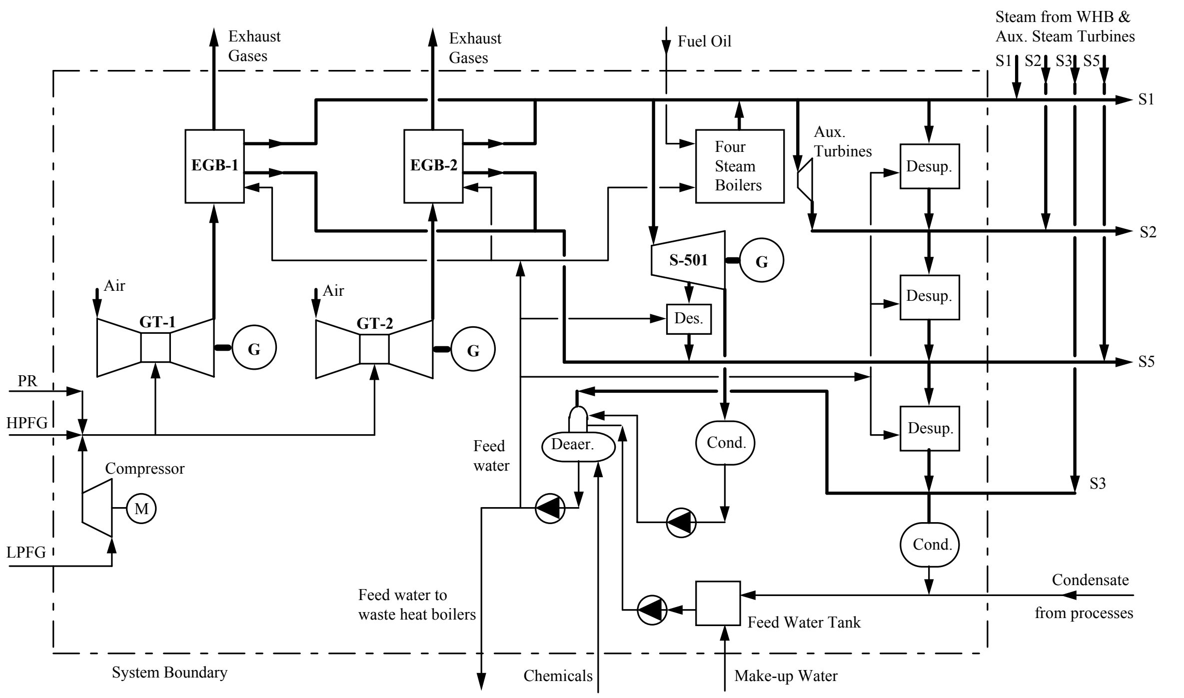

Fig. 9.1.1. Simplified diagram of the combined-cycle cogeneration system.

Table 9.1.1. Steam grades used in the refinery.

Grade designation	Pressure kPa (absolute)	Temperature °C
S1	4240	410
S2	1350	320
S3	370	150
S5	470	160

The system consists of the following main components (Fig. 9.1.1):

- Two gas-turbine electricity generators (GT-1, GT-2).
- Two exhaust-gas boilers (EGB-1, EGB-2) recovering heat from the gas turbine flue gases.
- One steam-turbine electricity generator (S-501).
- Four steam boilers.

A brief description of these components follows.

Gas-turbine electricity generators. They have a nominal electricity production capacity of 17 MW each. They can operate on Diesel oil, fuel gas, propane, or a combination of fuel gas and propane. Diesel oil is normally used for start-up only.

Exhaust-gas boilers. Each boiler has a nominal production capacity of 30 t/h of high pressure steam (S1) and 7 t/h of low pressure stream (S5). There is no supplementary firing.

Steam-turbine electricity generator. It uses high pressure steam (S1) and has a nominal capacity of 16 MW.

Steam boilers. They use fuel oil and produce high pressure steam (S1). There are two boilers with a nominal capacity of 30 t/h each, and two boilers with a nominal capacity of 60 t/h each. Thus, the total steam capacity of the four boilers is 180 t/h.

The main components are served by auxiliary equipment such as a compressor to increase the pressure of low-pressure fuel gas from 370 kPa to 2300 kPa, a propane vaporizer, water demineralization units, condensate collection and treatment units, etc.

9.1.2 Primary energy sources

The energy sources considered as primary for the energy system are the following.

Electricity supply from the utility grid. Currently, the electricity production capacity of the energy system is higher than the needs of the refinery and gives the possibility of exporting electricity to the utility grid. In special circumstances the refinery may need to import electricity from the grid. Thus, the refinery is connected to the grid for safety and for the possibility of exporting electricity.

Fuel gas (FG). It is the largest primary energy source for the refinery. It is a by-product of the refinery process units: it consists of light hydrocarbons (methane to butane) and a small percentage of hydrogen (about 5% by volume). Fuel gas is used in fired heaters for process and in the two gas turbines. It cannot be stored. A small inventory (depending on pressure) in the accumulation vessels and piping distribution system does exist, but there is no storage of FG. Thus, the rate of consumption must be equal to the rate of production. Any unbalance is automatically directed to the flares, where it is burned. The amount of FG burned in the flares is a total loss for the refinery that must be avoided. FG is available at two pressure levels: high-pressure and low-pressure.

Fuel oil (FO). It is the second largest primary energy source for the refinery. It is commercial industrial grade fuel oil (900 kg/m^3, 370 cSt at 50°C max) of special low sulfur content (0.7% by weight, maximum) because of strict environmental regulations in the area. Fuel oil is used in the fired heaters (if fuel gas is not sufficient) and in the four steam boilers.

Propane. It is used only as a supplement of FG burned in the gas turbines, if such a need arise or if economics favor it. Propane is a sellable final product. Its use as a fuel in the refinery depends on propane storage availability and its selling price. Use of propane in the gas turbines results in diverting FG from the gas turbines to fired heaters, substituting FO. Thus, there is actually a trade-off between FO (which also a sellable product) and propane, and the use of one or the other depends on their selling price. The propane used as fuel in the refinery is pumped from liquid storage tanks to a vaporizer. Propane vapor is mixed with the fuel gas stream feeding the gas turbines, if needed.

9.1.3 Energy conversion

The various fuels are converted to heat, steam and electricity. Process heat needs are covered by fired heaters using FG and/or FO or by steam. Steam is produced by steam boilers, and by waste heat boilers in the process units as well as in the cogeneration system. In order to satisfy the variety of steam needs of the process units in the most economical way, the refinery uses four different grades of steam with properties as given in Table 9.1.1. If the quantity of steam directly produced at a certain grade is not sufficient, then it is supplemented by throttling and temperature reduction of a higher grade steam (desuperheating) which, of course, causes an exergy destruction and consequently must be avoided whenever possible.

9.1.4 The need for operation optimization

As described above, the energy needs of the refinery can be satisfied by several primary energy sources through various energy conversion systems. This flexibility presents an excellent opportunity for optimization of the energy supply-conversion-utilization system. Important considerations in this optimization are the following:

- Electricity can be produced (within certain limits) either by the gas turbines or by the steam-turbine generator. The optimum load distribution is requested.
- Gas-turbine generators produce electricity and steam simultaneously. Thus, increased gas turbine level of electricity production results in an increase of steam availability, reducing the required production of steam by the steam boilers.
- Increasing the level of electricity production by the steam-turbine generator results in reduced steam availability, thus increasing the required production of steam boilers.
- Electricity can be exported to the utility grid (depending on availability and prices). The quantity of the exported electricity affects the operation of the gas turbines, steam turbine and boilers.
- Production and consumption of the various steam grades must be kept in balance to avoid degrading steam of higher levels to lower levels at a loss (i.e. without production of mechanical work).

The complicated structure of the system and the interdependency of its components make it impossible to determine the optimum mode of operation at various conditions by a heuristic approach or by past experience only. Therefore, it is necessary to develop an optimization procedure based on a careful analysis of the system, which will take into consideration the technical and economic parameters pertinent at a certain time period.

9.1.5 The optimization objective

Minimization of the capital and operating cost at any instant of time is selected to be the optimization objective. It is written:

$$\begin{aligned} \min F = \sum_r (\dot{C}_a + \dot{C}_m + \dot{C}_p)_r + c_{LF}\dot{m}_{LF} + c_{HG}\dot{m}_{HG} + c_{LG}\dot{m}_{LG} + c_{PR}\dot{m}_{PR} \\ + c_D\dot{m}_D + c_{el}\dot{W}_b - p_{el}\dot{W}_s + c_{c1}\dot{V}_{c1} + c_{w1}\dot{V}_{w1} + c_{cw}\dot{V}_{cw} + c_{chf}\dot{V}_{w3} \end{aligned} \tag{9.1.1}$$

The symbols are explained in the nomenclature. It is assumed that the operation mode at a certain instant of time does not affect and it is not affected by the operation mode at another instant of time.

By thermodynamic analysis of the system, the interrelationships among operating variables (pressures, temperatures, flow rates, power consumed or produced, etc.) have been obtained in the form of a system of equations. The difference between the number of variables and the number of equations (degree of freedom) is four. Consequently, Four of the variables can be treated as independent decision variables of the optimization problem. The following variables are selected as independent:

$$\mathbf{x} = (\dot{W}_{SG}, \dot{W}_{G1}, \dot{W}_{G2}, \dot{m}_e) \tag{9.1.2}$$

There are inequality constraints imposed on the independent variables:

$$0.5 \le \dot{W}_{SG} \le 16.5\ \text{MW}, \qquad 6 \le \dot{W}_{G1}, \dot{W}_{G2} \le 17\ \text{MW}, \qquad 0 \le \dot{m}_e \le 16.667\ \text{kg/s} \tag{9.1.3}$$

The net electric power produced by the cogeneration system is:

$$\dot{W} = \dot{W}_{SG} + \dot{W}_{G1} + \dot{W}_{G2} - \dot{W}_A \tag{9.1.4}$$

The total electric power supplied by the cogeneration system and the utility grid is:

$$\dot{W}_t = \dot{W} + \dot{W}_b - \dot{W}_s \tag{9.1.5}$$

The system analysis is supplemented by mathematical simulation of the main components and important auxiliary equipment. Performance specifications given by the manufacturer of each component or, in some cases, data collected by the refinery have been used to develop analytic correlations among important operating variables of components. Certain simplifying assumptions were inevitable whenever the available information was not sufficient.

9.1.6 Considerations on capital and operation expenses

The introduction of capital depreciation, maintenance and personnel costs in the objective function has an impact on the optimum point only if these costs can be expressed as functions of independent variables. Lack of sufficient data to develop the functions led, initially, to the decision to consider these expenses either constant (i.e. independent of the production level of a component) or sunk (zero). Such a simplification has the following consequence: the system produces extra electricity, which is sold to the utility grid even at an extremely low unit price of electricity (value of p_{el}). In order to avoid such a consequence, the following approach has been followed. Four main subsystems have been considered: fuel-oil boilers (r=1), steam-turbine generator (r=2), gas-turbine generator No. 1 with exhaust boiler (r=3), and gas-turbine generator No. 2 with exhaust boiler (r=4). The capital cost of the fuel-oil boilers is considered zero again, because they are considered fully depreciated. For the remaining subsystems it is written:

$$\dot{C}_{a2} = c_{a2}\,\dot{W}_{SG}, \qquad \dot{C}_{a3} = c_{a3}\,\dot{W}_{G1}, \qquad \dot{C}_{a4} = c_{a4}\,\dot{W}_{G2} \tag{9.1.6}$$

Each c_{ar} is a constant, which is estimated by taking into consideration the initial investment, the nominal capacity, as well as typical values for the life-time, the average availability and the load factor of the subsystem.

Maintenance and personnel costs are written as:

$$\dot{C}_{mpr} = (\dot{C}_m + \dot{C}_p)_r = c_{mpr}\,\dot{Y}_r \tag{9.1.7}$$

where

$$\dot{Y}_1 = \dot{m}_{sB}, \qquad \dot{Y}_2 = \dot{W}_{SG}, \qquad \dot{Y}_3 = \dot{W}_{G1}, \qquad \dot{Y}_4 = \dot{W}_{G2} \tag{9.1.8}$$

A rough estimate of the value of the parameter c_{mpr} is possible by means of available data.

This approach is still simplified, but it is more realistic than the initial one.

9.1.7 Description of the computer program

The optimization problem could be solved by the Functional Approach, which makes use of Lagrange multipliers. In the present work, the direct application of a mathematical programming algorithm has been used. The direct approach does not reveal the internal economy of the system, but it is less demanding from the point of view of system analysis. For the numerical solution, a computer program has been developed, which consists of the following parts.

Main program. It reads the values of the technical and economic parameters supplied by the user. It evaluates those variables that depend on the parameters but not on the independent variables. It calls the optimization algorithm and prints the results, i.e. the values of the independent variables and the objective function.

Optimization algorithm GRG2. It consists of a set of subroutines, which perform the optimization [Lasdon and Waren 1986]. It reads the initial set of values for the independent variables supplied by the user. It solves the optimization problem, i.e. it determines the optimum values of the independent variables. It prints the results (optimum point and messages regarding convergence). The algorithm is based on the generalized reduced gradient method and it is commercially available.

Constraints subroutine GCOMP. It is called by the optimization algorithm. It calls other subroutines or functions in order to determine the values of the inequality constraint functions and of the objective function for any given set of values of the independent variables.

Objective function FZ. It is a double precision function, which evaluates the objective function for any given set of values of the independent variables. It is called by the subroutine GCOMP.

Component simulation package. It is a set of double precision functions, which are called in order to determine the values of the operating variables of the main components. The functions constitute the mathematical simulation of the main components and important auxiliary equipment of the system.

File DSTEAM. It consists of a set of double precision functions, which evaluate thermodynamic properties of water and steam.

9.1.8 Numerical results

Results for typical load conditions

The usual practice in the refinery had been to distribute the electric load among the three main sources of electricity in proportion to their nominal capacity. For example, a typical condition is as follows:

$$\dot{W}_{SG} = 11\,\text{MW}, \qquad \dot{W}_{G1} = 12\,\text{MW}, \qquad \dot{W}_{G2} = 12\,\text{MW}, \qquad \dot{m}_e = 45\,\text{t/h}$$

with no electricity sold to the grid ($\dot{W}_s = 0$). By applying the optimization procedure described in the preceding sections, it is revealed that the optimum mode of operation is:

$$\dot{W}_{SG} = 5.58\,\text{MW}, \qquad \dot{W}_{G1} = 17\,\text{MW}, \qquad \dot{W}_{G2} = 17\,\text{MW}, \qquad \dot{m}_e = 50.36\,\text{t/h}$$

with an amount of electricity sold to the grid. The value of the objective function (total cost) at the optimum mode is by 13.75% lower than the value at the mode of usual practice.

Application of the optimization procedure leads to increased load of the gas-turbine generators, because they, together with the exhaust gas boilers, constitute cogeneration systems of high efficiency. Also, the mass flow rate of the extracted steam is increased for a similar reason: higher mass flow rate of extracted steam gives higher total efficiency of the steam-turbine generator as a system producing both electricity and heat (cogeneration).

Examples of Sensitivity Analysis

A sensitivity analysis has been performed with respect to important parameters. For example, the effect of the unit cost of electricity and fuel oil on the optimum values of the independent variables is shown in Figs. 9.1.2 and 9.1.3. It is noted that the nominal values of these parameters (i.e. the values that give the results presented in the preceding paragraph) are the following:

$$c_{el} = 0.035\ \text{Euro/kWh}, \qquad c_{LF} = 0.069\ \text{Euro/kg}$$

The effect of the unit cost of electricity purchased from the utility grid, c_{el}, has been studied. For unit price of electricity sold to the utility grid, p_{el}, equal to zero, this effect is depicted in Fig. 9.1.2, which reveals a critical value of c_{el} equal to approximately 0.01

Euro/kWh. Unit costs lower than the critical value drive the optimum operation point to the lower limit set on the gas- and steam-turbine power output, Eq. (9.1.3). For unit costs higher than the critical one and p_{el} equal to zero, the system produces enough electricity to cover the needs only. For p_{el} equal to its nominal value, the system produces extra electricity to cover the needs and sell to the grid. Consequently in this case, c_{el} does not have any effect on the optimum point, since there is no purchase of electricity from the grid.

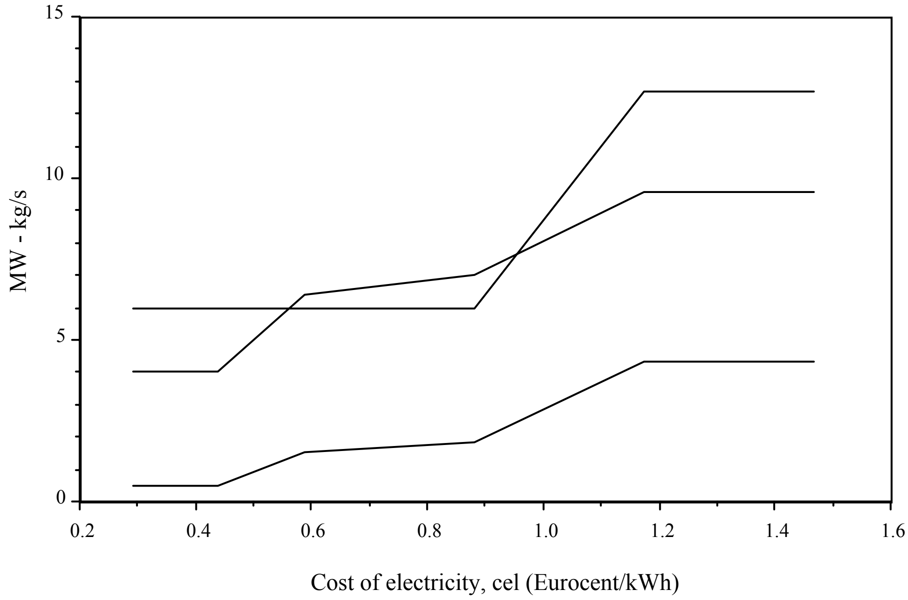

Fig. 9.1.2. Effect of unit cost of electricity purchased from the grid on the optimum operating point.

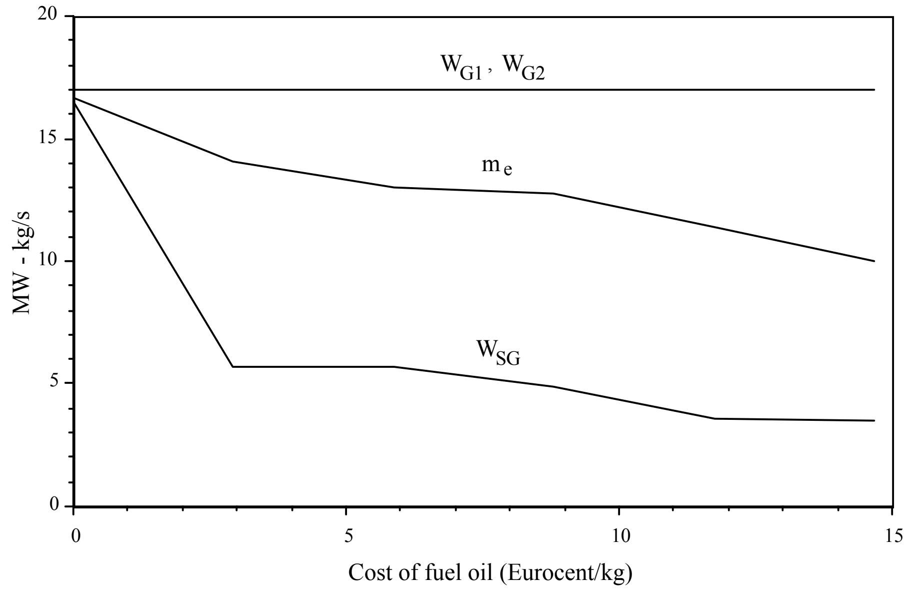

Fig. 9.1.3. Effect of unit cost of fuel oil on the optimum operating point.

Even though not shown here in order to save space, the sensitivity analysis reveals a critical value for p_{el} too. For values of p_{el} lower than the critical one, the system produces electricity equal to or less than the load (depending on the value of c_{el}). For values higher than the critical one, there is excess electricity sold to the grid.

An increase of fuel-oil unit cost does not affect the electricity produced by the gas turbines, but it has a decreasing effect on the steam-turbine power output (Fig. 9.1.3). Up to the value of 0.147 Euro/kg examined here, the load of the refinery is fully covered, but the excess electricity sold to the grid decreases continuously.

A note of caution: all costs are referring to the year 1990. In today's prices, the absolute values are expected to be higher, but this does not create any difficulty since the user can update the cost parameters.

The system operator can perform a sensitivity analysis with respect to any parameter that may be considered crucial. Very often, the sensitivity analysis is so revealing, that it may be more important than the solution of the optimization problem for a particular set of parameters.

9.1.9 Conclusions on the example

It has been demonstrated that the application of an optimization procedure to a complex system like the one studied here is very beneficial: if the common practice is replaced by the optimization procedure for setting the operation point of the system, a very significant reduction in operating expenses can be achieved with no need of additional investment. Every time the technical or economic conditions change, the user may update the values of the pertinent parameters and run the program again, in order to obtain the new optimum point very quickly.

Of course, the simplifying assumptions leave much room for further development and improvement of the procedure and the software. Also, in a further development, the limits of the system under optimization may be extended to include the refinery processes.

In this particular example, off-line optimization has been applied, which is satisfactory when the plant operates at nearly constant conditions for relatively long periods of time. For frequent changes of conditions (e.g. load), however, on-line optimization is necessary. For this purpose, crucial operating parameters are monitored, data reconciliation is performed, their values are fed into the optimization software, the results of which are sent to the control system of the plant in order for the optimal operating point to be set. On-line optimization requires fast simulation and optimization software. Application of neural networks, in particular for simulation, seems to be promising in this respect.

9.2. Thermoeconomic Design Optimization of a System

9.2.1 Description of the system and main assumptions

As an application example of design optimization, a cogeneration system will be used, which operates on natural gas and produces electricity and heat in the form of saturated steam [Frangopoulos 1994]. The system consists of a gas-turbine unit with regenerative air preheater, and a heat recovery steam generator (HRSG). Specifications of the system and the environment are given in Table 9.2.1

In order not to obscure the presentation, only major components are considered (Fig. 9.2.1) and certain simplifying assumptions are made:

(i) The air and combustion gases behave as ideal gases with constant specific heats.

(ii) For combustion calculations, the fuel is considered as methane (CH_4).
(iii) All components, except the combustion chamber, are adiabatic.
(iv) Pressure and temperature losses in the ducts connecting the components are neglected. However, a pressure drop due to friction is taken into consideration in the air preheater (both streams), combustion chamber and the HRSG.
(v) Mechanical losses in the compressor and turbine are negligible.

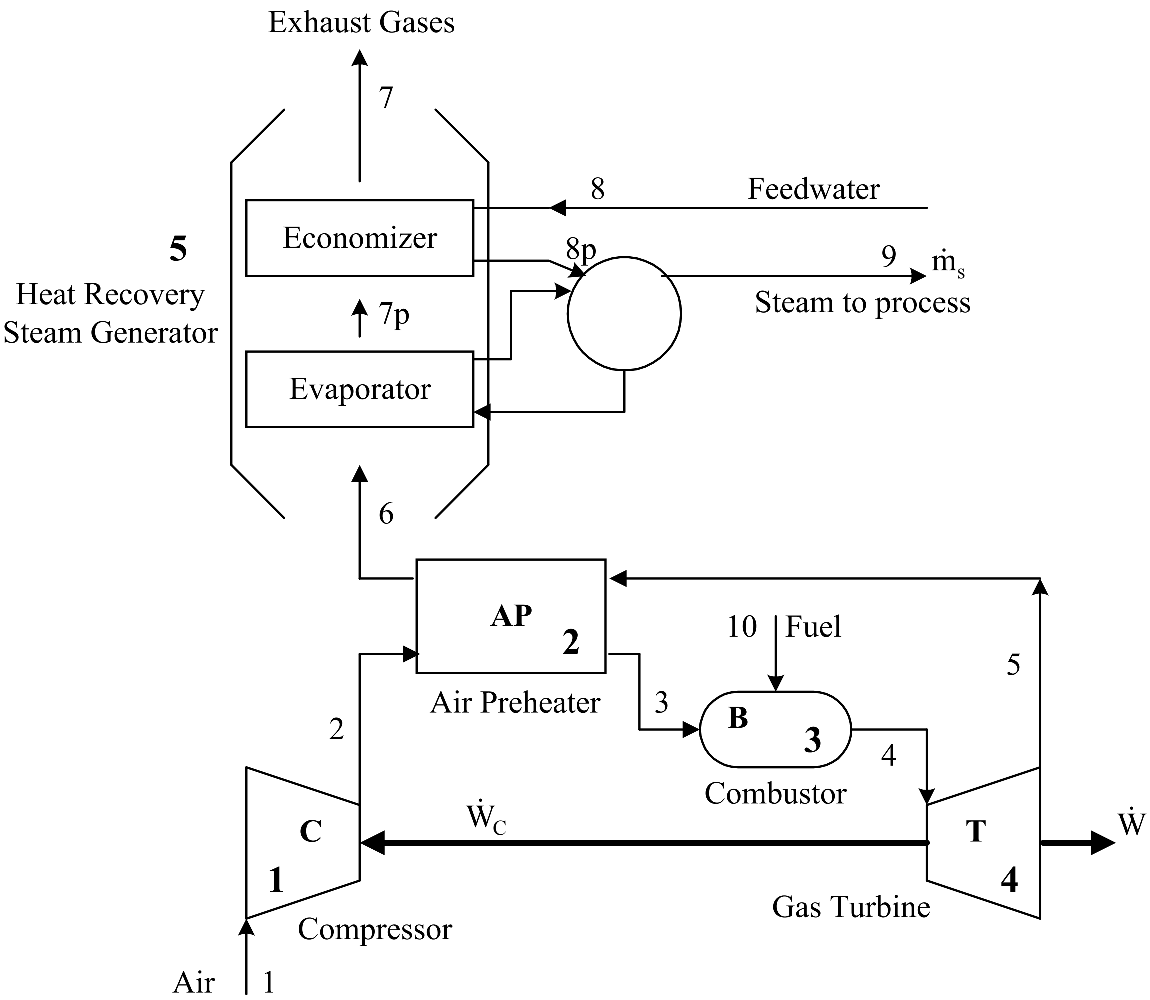

Fig. 9.2.1. Flow diagram of the gas-turbine cogeneration system.

9.2.2 Preliminary calculations

Using the data in Table 9.2.1 and tables with properties of water and steam, the following quantities are determined (numerical subscripts correspond to the points on the diagram of Fig. 9.2.1).

Steam temperature: $T_9 = T_{sat}(20 \text{ bar}) = 212.37°C$

Preheated water temperature: $T_{8p} = T_9 - \Delta T_{8p} = 197.37°C$

Table 9.2.1. Thermodynamic parameters for the system of Fig. 9.2.1.

Net shaft power:	$\dot{W} = 30\,\mathrm{MW}$	
Steam flow rate:	$\dot{m}_s = 14\,\mathrm{kg/s}$ (Fig. 9.2.1: $\dot{m}_8 = \dot{m}_9 = \dot{m}_s$)	
Steam condition:	p_9 = 20 bar, saturated	
Feedwater conditions:	p_8 = 20 bar	T_8 = 25°C
Temperature difference:	$\Delta T_{8p} \equiv T_9 - T_{8p} = 15\,\mathrm{K}$	
Reference environment:	p_0 = 1.013 bar	T_0 = 25°C
Other pressures and temperatures:	p_1 = 1.013 bar	T_1 = 25°C
	p_7 = 1.013 bar	T_{7min} = 100°C
Fuel properties (CH_4)		
Molar mass:	M_f = 16.043 kg/kmol	
Lower heating value:	H_u = 50000 kJ/kg	
Specific chemical exergy:	$\varepsilon_f^{CH} = 51850\,\mathrm{kJ/kg}$	
Conditions at the combustor inlet:	T_{10} = 25°C	

Properties of air and exhaust gas for compression and expansion calculations (ideal gas model):

c_{pa} = 1.004 kJ/kg·K	$\gamma_a = 1.40$	R_a = 0.287 kJ/kg·K
c_{pg} = 1.170 kJ/kg·K	$\gamma_g = 1.33$	R_g = 0.290 kJ/kg·K

Efficiency of the combustor : $\eta_B = 0.98$ (i.e. thermal losses 2%)

Overall heat transfer coefficient in the air preheater: U = 0.018 kW/m^2 K

Exit/inlet pressure ratios in components due to friction

Air preheater – air side:	r_{Aa} = 0.95
Air preheater – exhaust gas side:	r_{Ag} = 0.97
Combustor and HRSG:	$r_B = r_R$ = 0.95

Useful heat rate (product of the system):

$$\dot{Q}_s = \dot{m}_s (h_9 - h_8) = 14 \frac{\mathrm{kg}}{\mathrm{s}} (2797.2 - 106.6) \frac{\mathrm{kJ}}{\mathrm{kg}} = 37668\,\mathrm{kW} \tag{9.2.1}$$

Useful heat rate of the economizer:

$$\dot{Q}_{EC} = \dot{m}_s (h_{8p} - h_8) = 14 \frac{\mathrm{kg}}{\mathrm{s}} (840.8 - 106.6) \frac{\mathrm{kJ}}{\mathrm{kg}} = 10279\,\mathrm{kW} \tag{9.2.2}$$

Useful heat rate of the evaporator:

$$\dot{Q}_{EV} = \dot{Q}_s - \dot{Q}_{EC} = 27389\,\mathrm{kW} \tag{9.2.3}$$

9.2.3 Thermodynamic model of the system

Based on the aforementioned assumptions and preliminary calculations, a set of thermodynamic equations can be written, which constitutes the thermodynamic model of the system. For convenience, the equations are collected in Appendix A.

In the 21 equations of Appendix A, there are 47 quantities (pressures, temperatures, mass flow rates, heat transfer area, etc.). Of those, 21 are parameters, the values of which either are given in Table 9.2.1 or have been determined in the preceding section. The solution of the system of 21 equations can give the values of 21 more quantities. Consequently, there remain 5 quantities to be determined, namely: $r_C, \eta_C, \eta_T, T_3, T_4$

If the values of these 5 quantities are given, then Eqs. (A.1)-(A.17) can be applied one after the other to obtain the values of all the variables (see also note at the end of Appendix A), in addition to the parameters specified in Table 9.2.1 and § 9.2.2.

9.2.4 Economic model of the system

Analytic equations are available, which give the installed capital cost of each component of the system as a function of design characteristics. They are given in Appendix A: Eqs. (A.22)-(A.26). The annualized capital cost of each component, which includes depreciation and maintenance, is calculated by:

$$\dot{Z}_r = FCR \cdot \phi \cdot C_r \tag{9.2.4}$$

where

- C_r installed capital cost of component r,
- FCR annual fixed charge rate,
- ϕ maintenance factor.

The total annual cost for the system is given by:

$$\dot{Z} = \sum_{r=1}^{5} \dot{Z}_r + c_f \, \dot{m}_f \, H_u \, t \tag{9.2.5}$$

where

- c_f cost of fuel per unit of energy,
- t time period of operation during a year.

The values of parameters appearing in the cost model are given in Appendix A, Table A.1.

9.2.5 Thermoeconomic functional analysis of the system

Either energy or exergy can be the cost carrier, and the economic analysis can be either monetary or physical. Here, exergy with monetary economics will be applied. There are various methods to define the cost carriers. The functional approach will be used here (Subsection 6.3).

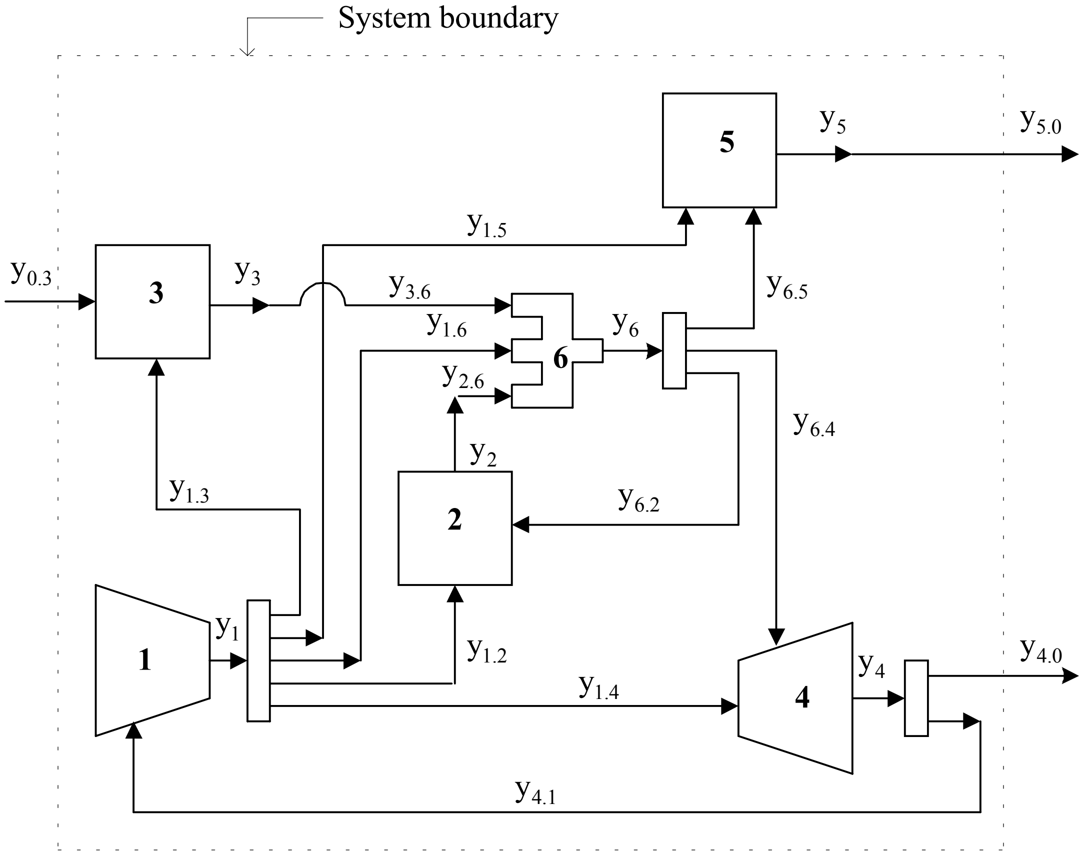

Fig. 9.2.2. Functional diagram of the system.

The function of the compressor is to increase the exergy of air from state 1 to state 2:

$$y_1 = \dot{m}_a(\varepsilon_2 - \varepsilon_1) = \dot{m}_a\left[\varepsilon_2^T - \varepsilon_1^T + R_a T_0 \ln\frac{p_2}{p_1}\right] \tag{9.2.6}$$

where

$$\varepsilon_2^T - \varepsilon_1^T = c_{pa}\left(T_2 - T_1 - T_0 \ln\frac{T_2}{T_1}\right) \tag{9.2.7}$$

To perform its function, the compressor uses shaft power, which comes from the turbine (unit 4):

$$y_{4\cdot1} = \dot{W}_C = \dot{m}_a c_{pa}(T_2 - T_1) \tag{9.2.8}$$

The mechanical exergy (due to pressure difference from the environment) is distributed to and consumed by all the other units according to the pressure drop in each unit:

$$y_{1.2} = \dot{m}_a R_a T_0\left(\ln\frac{p_2}{p_3} + \ln\frac{p_5}{p_6}\right) \tag{9.2.9}$$

$$y_{1.3} = \dot{m}_a R_a T_0 \ln \frac{p_3}{p_4} \tag{9.2.10}$$

$$y_{1.4} = \dot{m}_a R_a T_0 \ln \frac{p_4}{p_5} \tag{9.2.11}$$

$$y_{1.5} = \dot{m}_a R_a T_0 \ln \frac{p_6}{p_7} \tag{9.2.12}$$

The thermal exergy (due to temperature increase in the compressor) is combined with the thermal exergy coming from the air preheater and the combustor in the junction (unit 6, which is conceptual, i.e. it does not correspond to a real component of the plant):

$$y_{1.6} = \dot{m}_a \left(\varepsilon_2^T - \varepsilon_1^T \right) \tag{9.2.13}$$

The air preheater (unit 2) increases the thermal exergy of air:

$$y_2 = \dot{m}_a \left(\varepsilon_3^T - \varepsilon_2^T \right) \tag{9.2.14}$$

by using thermal exergy from exhaust gases:

$$y_{6.2} = \dot{m}_g \left(\varepsilon_5^T - \varepsilon_6^T \right) \tag{9.2.15}$$

The product of the air preheater is given to the junction:

$$y_{2.6} = \dot{m}_g \left(\varepsilon_3^T - \varepsilon_2^T \right) \tag{9.2.16}$$

The combustor (unit 3) increases the thermal exergy of the fluid from state 3 to state 4:

$$y_3 = \dot{m}_g \varepsilon_4^T - \dot{m}_a \varepsilon_3^T \tag{9.2.17}$$

by consuming fuel:

$$y_{0.3} = \dot{m}_f H_u \tag{9.2.18}$$

In Eq. (9.2.18) fuel energy appears instead of exergy. There is nothing wrong with this choice, provided that cost of fuel per unit of energy is used. The function of the combustor is given to the junction:

$$y_{3.6} = \dot{m}_g \varepsilon_4^T - \dot{m}_a \varepsilon_3^T \tag{9.2.19}$$

The turbine (unit 4) produces shaft power:

$$y_4 = \dot{W}_T = \dot{m}_g c_{pg} (T_4 - T_5) \tag{9.2.20}$$

by using mechanical exergy $y_{1.4}$ from the compressor, Eq. (9.2.11), and thermal exergy from the junction:

$$y_{6.4} = \dot{m}_g\left(\varepsilon_4^T - \varepsilon_5^T\right) \tag{9.2.21}$$

The function of the turbine is distributed to the compressor, $y_{4.1}$, Eq. (9.2.8), and to the environment as net power output:

$$y_{4.0} = \dot{W} \tag{9.2.22}$$

The heat recovery steam generator increases the exergy of water at state 8 to steam at state 9:

$$y_5 = \dot{m}_s(\varepsilon_9 - \varepsilon_8) \tag{9.2.23}$$

by using thermal exergy received from the junction:

$$y_{6.5} = \dot{m}_g\left(\varepsilon_6^T - \varepsilon_7^T\right) \tag{9.2.24}$$

The function of the boiler is one of the system products:

$$y_5 = y_{5.0} \equiv \dot{E}_s^Q \tag{9.2.25}$$

The function of the junction (unit 6) is to increase the thermal exergy of the working fluid from state 1 to the state of maximum temperature in the cycle, i.e. state 4. However only part of this increase is used, namely $\left(\varepsilon_4^T - \varepsilon_7^T\right)$, while the rest is rejected to the environment where it is destroyed. Since the functions are cost carriers, as it will be explained in the following, they must be defined so that there is no cost rejection to the environment (cost is transferred to the environment but through the useful products). For this reason, the function of the junction is defined as:

$$y_6 = y_{6.2} + y_{6.4} + y_{6.5} = \dot{m}_g\left(\varepsilon_4^T - \varepsilon_7^T\right) \tag{9.2.26}$$

Equations (9.2.6) – (9.2.26) define all the functions appearing in the functional diagram of Fig. 9.2.2.

It is useful to note that there is considerable flexibility in defining the functions and constructing the functional diagram of a system, provided certain fundamental rules are obeyed. The designer can use his own judgment and can introduce considerations pertinent to the particular applications.

The function distribution network, Fig. 9.2.2, distributes also the costs to the units and to the final products of the system. A cost balance is written for each unit considering a break-even operation:

$$\dot{Z}_r + \sum_{r'=1}^{5} c_{r'} y_{r'.r} = c_r y_r \tag{9.2.27}$$

The system of Eqs. (9.2.27) can be solved for the unit product costs, c_r. Equation (9.2.27) can be used not only with monetary costs but also with costs measured in terms of energy, exergy, etc. (physical economic approach).

9.2.6 Statement of the optimization problem

Minimization of the total cost rate of the system is selected as the optimization objective function:

$$\min_{\mathbf{x}} F = \sum_{r=1}^{5} \dot{Z}_r + c_f \dot{m}_f H_u \tag{9.2.28}$$

where $\mathbf{x} = (r_C, \eta_C, \eta_T, T_3, T_4)$

The reason why there are five independent variables has been explained in § 9.2.3. Any set of five variables can be selected as independent. The one selected here facilitates the calculations: the system of Eqs. (A.1) – (A.21) is diagonal, consequently it is solved one equation after the other with no iterations.

In addition to the equality constraints given in Appendix A, the following inequality constraints are imposed:

$$\begin{array}{llll} T_3 - T_2 \geq 0, & T_5 - T_3 \geq 0, & T_6 - T_2 \geq 0, & T_7 \geq 100°C \\ T_4 - T_3 \geq 0, & T_6 - T_9 \geq 0, & T_{7p} - T_9 \geq 0 & \end{array} \tag{9.2.29}$$

For the Functional Approach, in particular, the equations of Section 3 are applied with

$$\sigma = 5 \qquad \text{and} \qquad R = 6 \tag{9.2.30}$$

The system has two fixed products, and Eq. (6.9) is written explicitly here:

$$y_{3 \cdot 0} = \hat{y}_{3 \cdot 0} = \dot{W} \qquad\qquad y_{5.0} = \hat{y}_{5.0} = \dot{E}_s^{Q} \tag{9.2.31}$$

Equations (6.7) give each input to a unit as a function of the independent variables and the "product" of the unit ($\mathbf{x}_r$, y_r). Equations (9.2.6) – (9.2.26) are used to derive the analytic expressions for the functions $Y_{r \cdot r'}$. Also, the capital cost rates are expressed as functions of ($\mathbf{x}_r$, y_r):

$$\dot{Z}_r = Z_r\left(\mathbf{x}_r, y_r\right) \tag{9.2.32}$$

Examples of analytic expressions for $Y_{r \cdot r'}$ and $\dot{Z}_r$ are given in Appendix A: Eqs. (A.27) – (A.31).

The basic procedure to solve the optimization problem by the Functional Approach consists of the following steps:

1. Select an initial set of values for **x**.
2. Determine the values of y by the system of Eqs. (6.7) and (6.8).
3. Evaluate the Lagrange multipliers by Eqs. (6.14) and (6.17b, c, d).

4. Check Eqs. (6.17a). If they are satisfied to an acceptable degree of approximation, then stop. Otherwise, select a new set of values for **x** and repeat steps 2-4.

Numerical methods can be used for the solution of the usually nonlinear system of Eqs. (6.17a). If analytic derivatives can be formulated and infeasible points can be avoided, the procedure can be applied successfully. Otherwise, minimization of the Lagrangian, Eq. (6.15), with respect to **x** by means of a nonlinear programming algorithm can be more efficient. The second procedure has been followed with this problem.

9.2.7 Application of the modular approach

Although the system studied here is not very complex and detailed design characteristics of components are not required, the modular approach will be applied for demonstrative purposes. The components of the system of Fig. 9.2.1 correspond to the following modules of Fig. 5.8: (1) compressor, (2) combustor and turbine, (3) air preheater, (4) steam generator. The combustor and the turbine are considered as one module, because in this way iterations between components are avoided completely.

The variables, the parameters and the simulation model of each module are given in Appendix A. Whenever possible (as in this example), the equations of each module are written in diagonal form, in order to avoid internal iterations. It is reminded that the values of parameters, **p**, are selected by the designer and remain constant during the optimization procedure.

9.2.8 Numerical results

The optimization problem has been solved by three methods: (i) direct application of the GRG2 algorithm [Lasdon and Waren 1986], (ii) Thermoeconomic Functional Approach (TFA), and (iii) modular simulation and optimization. The results for the nominal set of parameter values (Tables 9.2.1 and A.1) are presented in Table 9.2.2. In addition, Tables 9.2.3 and 9.2.4 give the values of the functions, Lagrange multipliers and unit product costs at the optimum point, which are obtained by TFA. All three methods reach practically the same optimum point. The differences in the values of the independent variables are negligible (0.02 – 0.08%); they are due to numerical approximations and to the fact that the objective function is not very sensitive to the independent variables in the vicinity of the optimum point.

Table 9.2.2. Optimization results for the nominal set of parameter values.

Variable	Method		
	Direct use of GRG2	TFA	Modular
r_C	8.59730	8.59770	8.59050
η_C	0.84641	0.84650	0.84653
η_T	0.87886	0.87871	0.87878
T_3 (K)	912.77	913.14	912.93
T_4 (K)	1491.40	1491.97	1491.50
F ($/year)	$1.0426 \cdot 10^7$	$1.0426 \cdot 10^7$	$1.0426 \cdot 10^7$

Table 9.2.3. TFA: values of functions at the optimum point (in kW).

$y_1 = 27476$	$y_{1.2} = 695$	$y_{3.6} = 56292$
$y_2 = 18894$	$y_{1.3} = 437$	$y_{4.1} = 29846$
$y_3 = 56292$	$y_{1.4} = 16731$	$y_{6.2} = 20407$
$y_4 = 59846$	$y_{1.5} = 437$	$y_{6.4} = 45237$
$y_5 = 12745$	$y_{1.6} = 9176$	$y_{6.5} = 17028$
$y_6 = 82672$	$y_{2.6} = 18894$	

Table 9.2.4. TFA: values of Lagrange multipliers and unit product costs at the optimum point (in $\$/10^6$ kJ).

$\lambda_1 = 8.7621$	$c_1 = 8.8211$
$\lambda_2 = 7.7861$	$c_2 = 7.9552$
$\lambda_3 = 5.8668$	$c_3 = 5.8672$
$\lambda_4 = 7.7614$	$c_4 = 7.8158$
$\lambda_5 = 3.7305$	$c_5 = 10.007$
$\lambda_6 = 6.7467$	$c_6 = 6.7922$

9.2.9 Sensitivity analysis

In order to study the effect of certain parameters on the optimal solution, a sensitivity analysis is performed. The effect of any parameter in Tables 9.2.1 and A.1 can be studied. In general, economic parameters are more uncertain and therefore it is necessary to investigate their effect. As an example, the effect of fuel and capital expenses on the optimum design and on the value of the objective function is presented in Figs. (9.2.3), (9.2.4) and Table 9.2.5. In addition, the uncertainties defined in Subsection 8.1(B) can be evaluated.

It is interesting to note that, according to the results in Table 9.2.5, the change of optimum values of the independent variables due to an increase of the capital cost by 100% is of the same order of magnitude as the change due to an increase of the fuel price by 100%, but of the opposite sign. If both fuel price and capital cost increase simultaneously by the same factor, then the optimum design point remains the same, because multiplication of the objective function by the same factor does not change the optimal solution.

In addition to the sensitivity of the solution to parameter values, the sensitivity of the objective function to the independent variables in the vicinity of the optimum point is of interest also. It shows how much the objective function will deteriorate, if, for any reason, the design point does not coincide with the optimum one. According to Table 9.2.6, a departure from the optimum along the η_T axis has the highest effect on the objective function, while a departure along r_C has the lowest one.

Table 9.2.5. Sensitivity of the optimal solution to the fuel price and capital cost.

Variation of variable	Fuel price	Capital cost
	+ 100%	+ 100%
$\Delta r_C^* / r_C^*$ (%)	+ 13.76	– 13.75
$\Delta \eta_C^* / \eta_C^*$ (%)	+ 1.03	– 0.88
$\Delta \eta_T^* / \eta_T^*$ (%)	+ 0.80	– 0.84
$\Delta T_3^* / T_3^*$ (%)	– 2.39	+ 2.53
$\Delta T_4^* / T_4^*$ (%)	+ 0.66	– 0.60
$\Delta F^* / F^*$ (%)	+ 89.00	+ 9.21

Table 9.2.6. Sensitivity of the objective function to the independent variables: $\left(F - F^*\right)/F^*$, %.

Variable x_i	$\left(x_i - x_i^*\right)/x_i^*$, (%)		
	– 10	– 5	+ 5
r_C	0.834	0.269	**
η_C	9.448	3.520	**
η_T	19.854	7.711	**
T_3	8.508	3.885	**
T_4	**	**	14.05
** Infeasible points			

9.2.10 General comments derived from the example

The application of three methods for the optimization of thermal systems has been demonstrated through this example. All three approaches have been successful in the particular application.

The direct use of an optimization algorithm is the simplest way, because it requires the least effort in system analysis, but it gives no information about the internal economy of the system (physical and economic relationships among the components). Scaling of the variables and of the objective function is usually required in order to achieve convergence to the optimum point. On the other hand, no method of nonlinear optimization can guarantee convergence to the global optimum. For this reason, there is need to start the search from different initial points. If the same final point is reached, then we are more or less confident that this is the true optimum.

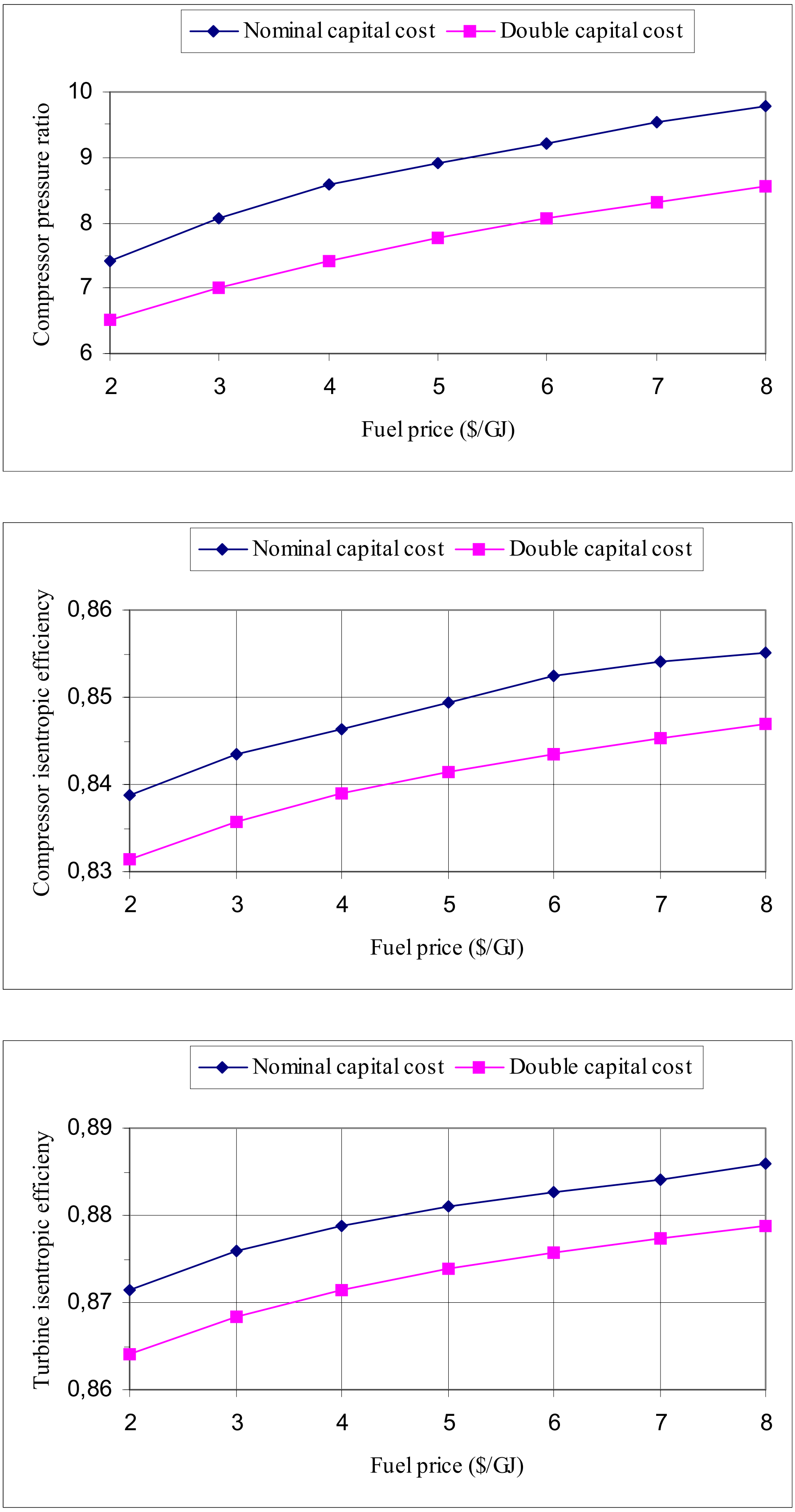

Fig. 9.2.3. Effect of fuel price and capital cost on the optimum values of r_C, η_C and η_T .

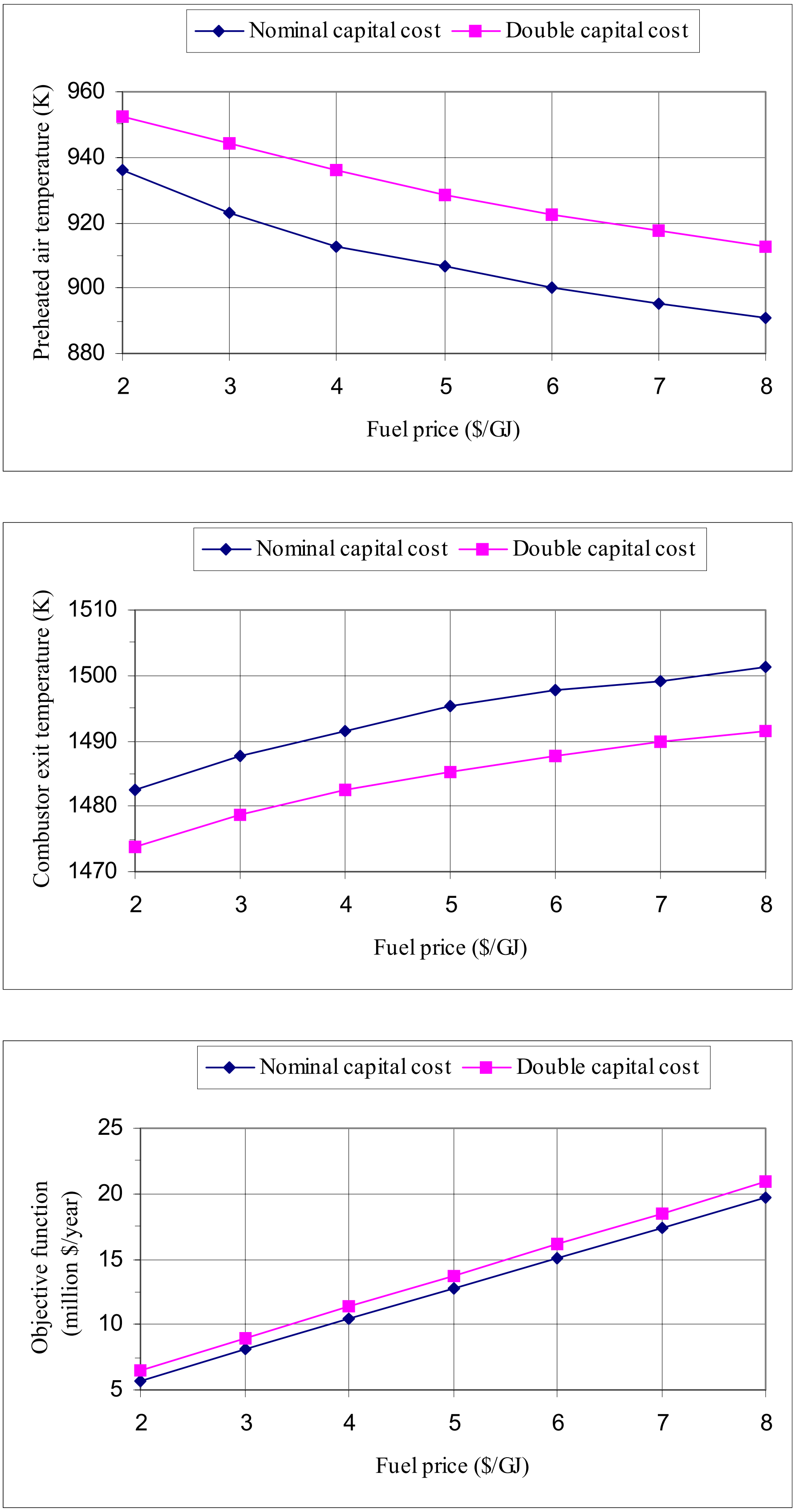

Fig. 9.2.4. Effect of fuel price and capital cost on the optimum values of T_3, T_4, and F.

9.3 Environomic Optimization of a System

9.3.1 Description of the system and main assumptions

A gas-turbine system operating on fuel oil will be used as an application example here [Frangopoulos 1992]. The system consists of a simple gas turbine unit equipped with a flue gas desulfurization unit (FGD) for SO_2 abatement (Fig. 9.3.1). It is considered that the plant operates at steady state and the electric power output, $\dot{W}_e$, is given. The operation of the FGD unit requires electricity, water and limestone ($\dot{W}_{el}$, $\dot{V}_w$ and $\dot{m}_{ls}$ in Fig. 9.3.1).

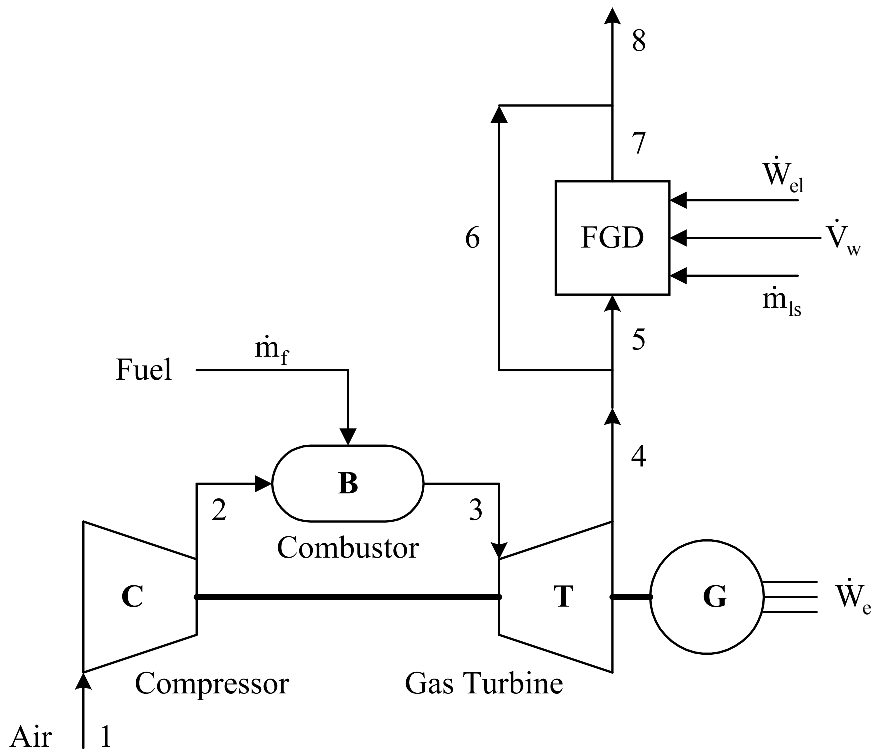

Fig. 9.3.1. Gas-turbine system with flue gas desulfurization unit.

The size and the capital cost of the desulfurization unit depend largely on the exhaust gas flow rate. Therefore, it is less expensive to desulfurize a partial flow at the maximum possible degree, $\delta_{S,max}$, than the total flow at a lower degree. This is why a by-pass of the FGD unit is shown in Fig. 9.3.1. If δ_S is the desirable degree of SO_2 abatement, then the mass and volume flow rates through the FGD unit are determined by the ratios:

$$\frac{\dot{m}_d}{\dot{m}_g} = \frac{\dot{V}_d}{\dot{V}_g} = \frac{\delta_S}{\delta_{S,max}} \tag{9.3.1}$$

where

$$\delta_S = \frac{\dot{m}_{Si} - \dot{m}_S}{\dot{m}_{Si}} \tag{9.3.2}$$

$\dot{m}_d, \dot{V}_d$ mass, volume flow rate of exhaust gases through the FGD unit (points 5 and 7 in Fig. 9.3.1),

$\dot{m}_g, \dot{V}_g$ total mass, volume flow rate of exhaust gases (points 3, 4 and 8 in Fig. 9.3.1),

$\dot{m}_{Si}$ initial mass flow rate of SO_2,

$\dot{m}_S$ final mass flow rate of SO_2 (after abatement).

For the particular system and fuel it is:

$$\dot{m}_{Si} = 2s\dot{m}_f \tag{9.3.3}$$

where

s mass fraction of sulfur in the fuel,

$\dot{m}_f$ mass flow rate of fuel.

9.3.2 Statement of the optimization problems

The system of Fig. 9.3.1, but without the HRSG, is optimized first with three different objectives, for comparison: two thermodynamic and one thermoeconomic. Next, the complete system (with the FGD unit) is optimized with an environomic objective. The two thermodynamic objectives are the maximization of the cycle efficiency:

$$\max_{\mathbf{x}_{th}} \eta = \frac{\dot{W}_e}{\dot{m}_f H_u} = \frac{\eta_C \eta_T \tau_3 \left[1-(\rho_B \rho_C)^{-1}\right] - (\rho_C - 1)}{\eta_C(\tau_3 - 1) - (\rho_C - 1)} \tag{9.3.4}$$

and the maximization of the net power density, defined as:

$$\max_{\mathbf{x}_{th}} w = \frac{\dot{W}_e}{\dot{m}_a c_p T_1} = \eta_T \tau_3 \left[1-(\rho_B \rho_C)^{-1}\right] - \frac{\rho_C - 1}{\eta_C} \tag{9.3.5}$$

where

$$\rho = r^{\frac{\gamma-1}{\gamma}} \tag{9.3.6}$$

η_C, η_T isentropic efficiency of compressor, turbine,

τ_3 temperature ratio: $\tau_3 = T_3/T_1$,

r_C, r_B, r_T compressor, combustor, turbine pressure ratio,

γ specific heat ratio: $\gamma = c_p/c_\upsilon$.

Both η and w increase continuously with η_C, τ_3, r_B and η_T. Consequently, the thermodynamic optimum value for each one of these variables is equal to 1, which is impractical, therefore realistic values will be assigned to these variables after the thermoeconomic or environomic problem is solved. The only independent variable left for the thermodynamic optimization problems is the compressor pressure ratio:

$$\mathbf{x}_{th} = r_C \tag{9.3.7}$$

As thermoeconomic objective, the minimization of the annual cost of owning and operating the system is selected:

$$\min_{\mathbf{x}_{te}} Z_{te} = Z_C + Z_B + Z_T + C_{f1} \tag{9.3.8}$$

where Z_C, Z_B and Z_T are the annualized capital costs of compressor, combustor and turbine, respectively, and C_{f1} is the annual cost of fuel.

The analysis of the system shows that there are five degrees of freedom. The following five variables are selected as independent:

$$\mathbf{x}_{te} = (r_C, \eta_C, r_B, \tau_3, \eta_T) \tag{9.3.9}$$

The environomic objective is selected similar to the thermoeconomic one, but it includes additional terms:

$$\min_{\mathbf{x}_{env}} Z_{env} = Z_{te} + Z_{FGD} + C_{el1} + C_{w1} + C_{ls1} + C_{S1} \tag{9.3.10}$$

where

Z_{FGD}	annualized capital cost of the FGD unit,
C_{el}, C_w, C_{ls}	cost of electricity, water and limestone consumed by the FGD unit,
C_{S1}	annual penalty imposed on the system for SO_2 emitted to the environment. C_{si} is a special case of C_S, which corresponds to no abatement ($\delta_S = 0$).

The capital costs of the compressor, combustor and turbine are given by the Eqs. (A.22), (A.24) and (A.25), respectively. The capital cost of the FGD unit is estimated by the equation:

$$C_{FGD} = c_1 \delta_S \dot{m}_{Si} + c_2 \dot{V}_d + c_3 \tag{9.3.11}$$

where c_1, c_2 and c_3 are constant cost coefficients. The annualized capital costs are calculated by Eq. (9.2.4). The remaining terms in Eqs. (9.3.8) and (9.3.10) are calculated by the equations

$$C_{f1} = c_f\, m_f \qquad\qquad C_{el1} = c_{el}\, k_{el}\, V_d \tag{9.3.12}$$

$$C_{w1} = c_w\, k_w\, V_d \qquad\qquad C_{ls1} = c_{ls}\, k_{ls}\, \delta_S m_{Si} \tag{9.3.13}$$

where

m_f	annual fuel consumption,
c_f, c_{el}, c_w, c_{ls}	unit cost of fuel, electricity, water and limestone, respectively,

k_{el}, k_w, k_{ls} specific consumption of electricity, water and limestone, respectively, by the FGD unit.

The first year penalty for emitted SO_2 is considered a linear function of the emitted quantity:

$$C_{S1} = c_S(1-\delta_S)m_{Si} \tag{9.3.14}$$

where c_S is the unit penalty on SO_2 emissions.

The degree of SO_2 abatement is included in the independent variables:

$$\mathbf{x}_{env} = (r_C, \eta_C, r_B, \tau_3, \eta_T, \delta_S) \tag{9.3.15}$$

The level of analysis (thermodynamic model) of the system is similar to the one of the preceding example (Appendix A). Details are not written here.

9.3.3 Numerical results and comments

The four optimization problems have been solved for the parameter values given in Table 9.3.1 and the results are presented in Table 9.3.2. As mentioned above, thermodynamic optimization requires η_C, τ_3, r_B and η_T to take the maximum possible value, ideally to be equal to 1. Since this is impossible, these variables are set equal to their optimum values of (i) the thermoeconomic optimization, and (ii) the environomic optimization problem. Thus, two different optimum values of r_C are obtained for each one of the two thermodynamic optimization problems, as shown in Table 9.3.2.

The environomic optimum values of all the independent variables are higher than the thermoeconomic optimum values. The thermoeconomic and environomic optima of r_C are in between the values corresponding to the maximum efficiency and the maximum net power density. The cycle efficiency, as a dependent variable, obtains a higher value with the environomic optimization than with the thermoeconomic optimization.

A more detailed presentation of this example appears in [Frangopoulos 1992]. Other examples of optimization with environmental considerations appear in [Frangopoulos and Boulmetis 1992, von Spakovsky and Frangopoulos 1994, and Agazzani et al. 1998].

Table 9.3.1. Parameter values for optimization of the system.

$\dot{W}_e$ = 100 MW_e	c_1 = $15\cdot10^6$ \$/(kg/s)
H_u = 42500 kJ/kg	c_2 = 56000 \$/(m^3/s)
T_1 = 293 K	c_3 = $9\cdot10^6$ \$
s = 0.025 kg S/kg fuel	c_{el} = 0.06 \$/kWh
$\delta_{S,max}$ = 0.95	c_w = 0.47 \$/m^3
c_f = $4\cdot10^{-6}$ \$/kJ	c_{ls} = 0.0257 \$/kg
c_S = 1.70 \$/kg SO_2	k_{el} = 0.0031 kWh/m^3
FCR = 0.13	k_w = $0.369\cdot10^{-4}$ m^3/m^3
ϕ = 1.04	k_{ls} = 1.56 kg/kg

Table 9.3.2. Optimization results.

Variable	Objective					
	max η		max w		min Z_{te}	min Z_{env}
r_C	25.83	28.1	10.39	10.82	15.22	16.14
η_C	*	#	*	#	0.8460	0.8555
r_B	*	#	*	#	0.9820	0.9839
T_3 (K)	*	#	*	#	1467.4	1478.6
η_T	*	#	*	#	0.8947	0.8993
δ_S	—	—	—	—	—	0.9500
η	0.4056	0.4202	0.3636	0.3750	0.3900	0.4034

* Equal to the thermoeconomic optimum value.
\# Equal to the environomic optimum value.

Note:
The last two application examples have to do with similar systems. However, differences in the size of systems and the time basis of economic analysis make the numerical results not to be comparable with each other.

APPENDIX A

Thermodynamic Model of the System of Subsection 9.2

$$T_2 = T_1\left(1+\frac{r_C^{k_a}-1}{\eta_C}\right) \quad (A.1) \qquad P_2 = r_C P_1 \quad (A.2)$$

$$P_3 = r_{Aa} P_2 \quad (A.3) \qquad P_4 = r_B P_3 \quad (A.4)$$

$$P_6 = P_7 / r_R \quad (A.5) \qquad P_5 = P_6 / r_{Ag} \quad (A.6)$$

$$r_T = P_4 / P_5 \quad (A.7) \qquad T_5 = T_4\left[1-\eta_T\left(1-r_T^{-k_g}\right)\right] \quad (A.8)$$

$$f = \frac{c_{pg}(T_4-T_0)-c_{pa}(T_3-T_0)}{H_u\eta_B - c_{pg}(T_4-T_0)} \quad (A.9) \qquad T_6 = T_5 - \frac{c_{pa}(T_3-T_2)}{(1+f)c_{pg}} \quad (A.10)$$

$$\dot{m}_a = \frac{\dot{W}}{(1+f)c_{pg}(T_4-T_5)-c_{pa}(T_2-T_1)} \quad (A.11) \qquad \dot{m}_f = f\,\dot{m}_a \quad (A.12)$$

$$\dot{m}_g = \dot{m}_f + \dot{m}_a \quad (A.13) \qquad T_7 = T_6 - \frac{\dot{Q}_s}{\dot{m}_g c_{pg}} \quad (A.14)$$

$$T_{7p} = T_6 - \frac{\dot{Q}_{EV}}{\dot{m}_g c_{pg}} \quad (A.15) \qquad \dot{W}_C = \dot{m}_a c_{pa}(T_2-T_1) \quad (A.16)$$

$$\dot{W}_T = \dot{m}_g c_{pg}(T_4-T_5) \quad (A.17) \qquad \Delta T_A = \frac{(T_6-T_2)-(T_5-T_3)}{\ln\dfrac{T_6-T_2}{T_5-T_3}} \quad (A.18)$$

$$A_A = \frac{\dot{m}_g c_{pg}(T_5-T_6)}{U\Delta T_A} \quad (A.19) \qquad \Delta T_{EC} = \frac{(T_{7p}-T_{8p})-(T_7-T_8)}{\ln\dfrac{T_{7p}-T_{8p}}{T_7-T_8}} \quad (A.20)$$

$$\Delta T_{EV} = \frac{(T_6-T_9)-(T_{7p}-T_9)}{\ln\dfrac{T_6-T_9}{T_{7p}-T_9}} \quad (A.21)$$

Symbols not explained in the text:

A_A heat transfer area of the air preheater,
f fuel to air mass ratio,

$$k = \frac{\gamma - 1}{\gamma} \qquad \text{where} \qquad \gamma = \frac{c_p}{c_\upsilon}$$

Economic Model of the System

Installed capital cost functions of components:

$$C_1 = \frac{c_{11}\dot{m}_a}{c_{12} - \eta_C} r_C \ln r_C \tag{A.22}$$

$$C_2 = c_{21} A_A^{0.6} \tag{A.23}$$

$$C_3 = \frac{c_{31}\dot{m}_g}{c_{32} - r_B}\left[1 + \exp(c_{33}T_4 - c_{34})\right] \tag{A.24}$$

$$C_4 = \frac{c_{41}\dot{m}_g}{c_{42} - \eta_T} \ln r_T \left[1 + \exp(c_{43}T_4 - c_{44})\right] \tag{A.25}$$

$$C_5 = c_{51}\left[\left(\frac{\dot{Q}_{EC}}{\Delta T_{EC}}\right)^{0.8} + \left(\frac{\dot{Q}_{EV}}{\Delta T_{EV}}\right)^{0.8}\right] + c_{52}\dot{m}_s + c_{53}\dot{m}_g^{1.2} \tag{A.26}$$

Table A.1. Nominal values of cost parameters (year of reference: 1992).

$t =$ 8000 h/year	$c_{21} =$ 2290.0 \$/m$^{1.2}$	$c_{42} = 0.92$
$c_f =$ $4 \cdot 10^{-6}$ \$/kJ	$c_{31} =$ 25.6 \$/(kg/s)	$c_{43} = 0.036$ K^{-1}
FCR = 0.182 (year)$^{-1}$	$c_{32} =$ 0.995	$c_{44} = 54.4$
$\phi =$ 1.06	$c_{33} =$ 0.018 K^{-1}	$c_{51} =$ 3650 \$/(kW/K)$^{0.8}$
$c_{11} =$ 39.5 \$/(kg/s)	$c_{34} =$ 26.4	$c_{52} =$ 11820 \$/(kg/s)
$c_{12} =$ 0.9	$c_{41} =$ 266.3 \$/(kg/s)	$c_{53} =$ 658 \$/(kg/s)$^{1.2}$

Examples of $Y_{r \cdot r'}(\mathbf{x}_{r'}, y_{r'})$ and $Z_r(\mathbf{x}_r, y_r)$.

$$y_{4 \cdot 1} = \frac{c_{pa}(T_2 - T_1)}{\varepsilon_2 - \varepsilon_1} y_1, \tag{A.27}$$

$$y_{0.3} = \frac{f H_u}{(1+f)\varepsilon_4^T - \varepsilon_4^T} y_3 \tag{A.28}$$

$$y_{1.4} = \frac{R_a T_0 \ln(1/r_T)}{(1+f)c_{pg}(T_4 - T_5)} y_3, \tag{A.29}$$

$$Z_1 = \frac{a_{11} r_C \ln r_C}{(c_{12} - \eta_C)(\varepsilon_2 - \varepsilon_1)} y_1 \tag{A.30}$$

where $$a_{ri} = FCR \cdot \phi \cdot c_{ri} \tag{A.31}$$

Modular Formulation of the Problem

Module 1: Compressor

Parameters and variables:

$\mathbf{p}_1 = (P_1, T_1, k_a)$, $\quad \mathbf{x}_1 = (r_C, \eta_C)$, $\quad \mathbf{y}_{1i} = (\varnothing)$, $\quad \mathbf{y}_1 = (P_2, T_2)$, $\quad \mathbf{w}_1 = (\varnothing)$

Simulation model: Eqs. (A.1), (A.2).

Module 2: Combustor and turbine

Parameters and variables:

$\mathbf{p}_2 = (T_0, T_1, P_7, c_{pa}, c_{pg}, k_g, H_u, \eta_B, r_{Aa}, r_{Ag}, r_B, r_R)$

$\mathbf{x}_2 = (\eta_T, T_3, T_4)$, $\quad \mathbf{y}_{2i} = (P_2)$ $\quad \mathbf{y}_2 = (\dot{m}_a, \dot{m}_f, \dot{m}_g, T_5)$ $\quad \mathbf{w}_2 = (P_4, P_5, r_T, f)$

Simulation model: $P_4 = r_{Aa} r_B P_2$ $\qquad P_5 = \dfrac{P_7}{r_{Ag} r_R}$

Eqs. (A.7) – (A.9) and (A.11) – (A.13).

Module 3: Air preheater

Parameters and variables:

$\mathbf{p}_3 = (c_{pa}, c_{pg}, U)$, $\quad \mathbf{x}_3 = (T_3)$

$\mathbf{y}_{3i} = (T_2, T_5, f, \dot{m}_g)$, $\quad \mathbf{y}_3 = (T_6, A_A)$, $\quad \mathbf{w}_3 = (\Delta T_A)$

Simulation model: Eqs. (A.10), (A.18) (A.19).

Module 4: Heat recovery steam generator

Parameters and variables:

$\mathbf{p}_4 = (T_{8p}, T_9, \dot{Q}_R, \dot{Q}_{ec}, \dot{Q}_{ev}, c_{pg})$, $\quad \mathbf{x}_4 = (\varnothing)$

$\mathbf{y}_{4i} = (T_6, \dot{m}_g)$, $\quad \mathbf{y}_4 = (T_7, T_{7p}, \Delta T_{ec}, \Delta T_{ev})$, $\quad \mathbf{w}_4 = (\varnothing)$

Simulation model: Eqs. (A.14), (A.15) (A.20), (A.21).

APPENDIX B

Sources of Optimization Software

Software packages

The continuously increasing interest in applying optimization not only in research but also in practical problems gave the impetus for development of appropriate software, which is commercially available or, in certain cases, is given free of charge. A very good reference is the guide by Moré and Wright (1993), which is available also on-line in the *NEOS Server* listed below. For convenience, a list of software packages is given here; it is not comprehensive and no attempt is made to make recommendations. Related information is given also in the books by Papalambros and Wilde (2000), Floudas (1995), Reklaitis et al. 1983.

Various software packages, such as *Excel, Lotus* and *QuatroPro* use the GRG algorithm for solution of optimization problems. The particular version of the GRG algorithm is provided by Frontline Systems (www.frontsys.com)

DOT (Design Optimization Tool)
Provided by: Vanderplaats R&D (www.vrand.com).
It contains general purpose nonlinear programming codes designed to interface with simulation analysis programs.

EASY-OPT
Provided by: K. Schittkowski
(www.uni-bayreuth.de/departments/math/~kschittkowsky/easy_opt)
It can solve general nonlinear programming, least squares, min-max, and multicriteria optimization problems interactively under the Microsoft Windows platform.

Harwell Subroutine Library
Provided by: www.dci.clrc.ac.uk
It is a suite of ANSI Fortran 77 subroutines and Fortran 90 modules for scientific computation, including modules for optimization.

IMSL (International Mathematical and Statistical Libraries)
Provided by: Visual Numerics (www.vni.com)
It was initially created in the late 1960s for use in business, engineering and sciences. It has been fully modernized and contains many algorithms including Schittkowski's SQP.

iSIGHT
Provided by: Engineous Software (www.engineous.com)
It is an optimization package based on a graphics environment with its early motivation coming from artificial intelligence techniques.

MATLAB Optimization Toolbox
Provided by: Mathworks (www.mathworks.com)
It includes unconstrained and SQP algorithms.

Mathematica

Provided by: Wolfram Research (www.wolfram.com)
It includes unconstrained and SQP algorithms.

NEOS (Network-Enabled Optimization System Server

Provided by: Optimization Technology Center of Argonne National Laboratory (www.mcs.anl.gov/otc)
It can be used for solving optimization problems remotely over the Internet.

SNOPT

Provided by: Systems Optimization Laboratory of Stanford University (www.stanford.edu/group/SOL/)
It is, perhaps, the most widely used and robust SQP code.

Internet sites

A search with keywords over the Internet is perhaps the best way to obtain updated information on software and algorithms. As a starting point, a few addresses are given below with a note of caution, since Internet addresses change frequently.

www.aemdesign.com/

It provides information about the FSQP method.

www.aero.ufl.edu/~issmo

The International Society for Structural and Multidisciplinary Optimization.
It provides links to research and events related to optimization.

www.me.washington.edu/~asmeda

ASME Design Automation Committee.
It provides links to research and events related to design optimization.

http://ode.engin.umich.edu/links.html

Optimal Design Laboratory, University of Michigan.
It maintains a list of Internet sites of special interest for design optimization.

www-unix.mcs.anl.gov/~leyffer/solvers.html

It provides information about optimization algorithms for nonlinear and mixed integer-nonlinear optimization problems based on the “filter SQP” method.

www-unix.mcs.anl.gov/~leyffer/

It provides information and results of comparison of various optimization algorithms.

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