

## A Brief Review of Methods for the Design and Synthesis Optimization of Energy Systems

Christos A. FRANGOPOULOS\*  
National Technical University of Athens  
Dept. of Naval Architecture and Marine Engineering  
Heroon Polytechniou 9, 157 73 Zografou, Greece.  
Tel: +30-210-7721108, Fax: +30-210-7721117  
E-mail: caf@naval.ntua.gr

Michael R. von SPAKOVSKY  
Virginia Polytechnic Institute and State University  
Mechanical Engineering Department,  
Blacksburg, VA 24061, USA.  
Tel: +1-540-2316684, Fax: +1-540-2319100,  
E-mail: vonspako@vt.edu

Enrico SCIUBBA  
Università di Roma 1 "La Sapienza"  
Dipartimento di Meccanica ed Aeronautica  
Via Eudossiana 18, 00185 Roma, Italy.  
Tel: +39-06-44585244, Fax: +39-06-4881759  
E-mail: enrico.sciubba@uniroma1.it

### Abstract

The optimization of energy systems is of crucial importance for a rational use of natural and economic resources and for minimizing their adverse effects on the environment. Optimizing such systems may be considered at three levels: synthesis (configuration), design (component characteristics), and operation. The first two of these levels are examined in this article. After a discussion on the uniqueness of the solution and the possibility of finding this solution, the principal approaches and methods for solving the optimization problem are described in brief.

*Key words: thermoeconomics, design optimization of energy systems, synthesis optimization of energy systems, artificial intelligence, genetic algorithms, mathematical programming, decomposition*

### 1. Introduction

When the energy needs of a group of consumers of any size (house, city, industrial unit, region, etc.) are identified, questions such as the following arise:

- 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, performance, 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?

The best or 'optimum' system is the one that satisfies a criterion of optimality, i.e. the one that minimizes (or maximizes) an objective function. Three levels of optimization are identified: (A) *synthesis*, implying the set of components appearing in a system and their interconnections, (B) *design*, implying the technical specifications of the components and the properties of sub-

\* Author to whom all correspondence should be addressed.

stances flowing throughout the system at the nominal load, and (C) *operation*, implying the operating properties of components and substances under specified conditions. The complete optimization problem is 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?*

Level C, which appears when the synthesis and design of a system are given, is not the subject of this article, but the interested reader can find information in the literature, e.g., (Bausa and Tsatsaronis 2001, Frangopoulos et al. 1996, Olsommer et al. 1999).

## **2. Discussion on the Uniqueness of the Solution of the Synthesis and Design Optimization Problem and on the Possibility of finding this Solution**

In mathematical optimization, the best system is the one that minimizes (or maximizes) an objective function. Let us assume that minimization of the total cost is the objective and that the optimization problem has a solution, i.e. a system has been determined that satisfies the objective. Is this indeed the solution sought or must one also compare the performance of this system with the performance of other (non-optimal) systems based on other points of view, e.g., maintainability or environmental effects? There may be cases when such a comparison shows that the 'optimal' with respect to the cost of the system is not at all good when these other points of view are considered (attempts to translate other aspects into cost are made but there may still be aspects that cannot be handled in this way). Multi-objective optimization is an attempt to correct such deficiencies. However, the solution then depends on subjective weighting factors or additional criteria. The point of all this is that the optimal solution may not be unique and is 'optimal' only in the strict mathematical sense. Thus, even if the design procedure can be automated, expert human intervention is needed to evaluate the results and reach a final decision.

Another issue is the following. In the usual design process of an energy system, the designer uses knowledge and experience to select the type, configuration and technical characteristics of a workable system (i.e. a system that is technically feasible and satisfies a given set of needs), which he/she then evaluates for its technical and economic performance and for ways of improving it. If the system synthesis (type and configuration) is given, the decisions to be taken are of a rather quantitative nature. If, however, the synthesis is not given, in addition to quantita-

tive decisions there is need for many qualitative decisions, which may be non-deterministic. In such a case, innovation and creativity play a vital role. Given the multitude of energy system types and the variations in each type, one may question whether it is ever possible to replace the experienced designer's mental process with an algorithm consisting of a set of formulae and rules. On the other hand, in today's complex world, this same multitude of types and variations makes it rather impossible even for an experienced designer to evaluate all possible alternatives. Consequently, an automated procedure, if properly used, can be of invaluable help to the designer.

Several methods have been developed for the synthesis optimization of processes and systems. Some of these are applicable only to particular classes of systems (e.g., heat exchanger networks). Other methods are applied to more complex energy systems. However, up until now there has been no single method that can tackle the synthesis optimization problem in all its generality and completeness. The field is, thus, still open to research.

## **3. Approaches to the Optimal Synthesis of Energy Systems**

The various methods that have appeared in the literature on the optimal synthesis of energy systems can be classified into three groups:

- (a) Methods based on heuristics and evolutionary search.
- (b) Methods attempting to reach pre-determined targets, which have been identified by the application of physical rules.
- (c) Methods starting with a superstructure, which is reduced to the optimal configuration.

In class (a), rules based on engineering experience and on physical concepts (e.g., exergy) are applied to generate feasible configurations, which are subsequently improved by applying a set of evolutionary rules in a systematic way. These rules may come from special techniques, such as exergy analysis. Artificial Intelligence and Expert Systems have proven effective in generating appropriate configurations. For each acceptable configuration, a figure of merit or performance indicator is evaluated (e.g., efficiency, cost, etc.) and the system with the best performance is selected. The best of a certain set of configurations, however, does not guarantee that the optimal configuration has been revealed. In most cases, though, at least a near-optimal configuration has been obtained (Kott et al. 1989, Sciubba 1998, Sciubba and Melli 1998).

In class (b), principles from thermodynamics and other physical sciences are applied to obtain targets for the optimal system configuration. These targets can correspond to upper or lower bounds on the best possible configuration and provide vital information for improvement of existing configurations. In addition, many configurations are excluded from further investigation, thus reducing the search space for the best system. If the physical target is the optimization objective (e.g., minimization of energy utilization), then these methods provide the solution to the optimization problem. However, if the optimization objective is economic, e.g., minimization of the total cost, then these methods are not very appropriate. Attempts have been made to introduce economics at a second level, but the whole approach is mathematically non-rigorous and, consequently, the configuration obtained may be non-optimal (Linnhoff et al. 1982, Linnhoff 1989).

In class (c), a superstructure is considered with all the possible (or necessary) components and interconnections. An objective function is specified and the optimization problem is formulated. The solution of the optimization problem gives the optimal system configuration, which, inevitably, depends on (and is restricted by) the initial superstructure. The main advantages of such an approach are that it can work with any objective function and that it automatically reveals the optimal system configuration. The difficulty with these methods is that the size of the optimization problem may be such that the available mathematical optimization algorithms may not be capable of a rigorous solution. Thus, the need arises for advances in optimization theory and algorithms. It goes without saying that the methods of class (c) can find the optimal configuration only out of those represented in the superstructure (Olsommer et al. 1999, Floudas 1995, Frangopoulos 1990, Munoz and von Spakovsky 2000, 2001a, 2001b).

It should be noted that the distinction among the three classes may not be so clear-cut. For example, the targets of class (b) can serve as heuristics or rules in class (a) and they can be embedded in the optimization procedures of class (c) to the benefit of the whole process.

#### 4. Mathematical Statement of the Complete Optimization Problem

The objective function of the complete optimization problem (i.e. synthesis, design, and operation) is written in the general form:

$$\min_{\mathbf{x}, \mathbf{w}, \mathbf{z}} \text{imize } F(\mathbf{x}, \mathbf{w}, \mathbf{z}) \quad (1)$$

subject to the constraints

$$h_i(\mathbf{x}) = 0, \quad i = 1, 2, \dots, I \quad (2)$$

$$g_j(\mathbf{x}) \leq 0, \quad j = 1, 2, \dots, J \quad (3)$$

where

- x** set of independent variables for operation optimization (load factors of components, mass flow rates, pressures and temperatures of streams, etc.),
- w** set of independent variables for design optimization (nominal capacities of components, geometry, mass flow rates, pressures and temperatures of streams, etc.),
- 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.

$h_i(\mathbf{x})$  equality constraint functions, which constitute the simulation model of the system and are derived by an analysis of the system (energetic, exergetic, economic, etc.),

$g_j(\mathbf{x})$  inequality constraint functions corresponding to design and operation limits, state regulations, safety requirements, etc.

Several objectives pertinent to energy systems can be written in the form of Eq. (1). For example,  $F$  can be the fuel consumption, exergy destruction, annualized cost of owning and operating the system, life-cycle cost (including environmental considerations, if needed), etc. Multi-objective optimization can also be written in the form of Eq. (1), but only if the various objectives are combined into one objective function by means of weighting factors.

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

$$\min_{\mathbf{x}, \mathbf{w}} \text{imize } F_d(\mathbf{x}, \mathbf{w}) \quad (1)_d$$

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

$$\min_{\mathbf{x}} \text{imize } F_{op}(\mathbf{x}) \quad (1)_{op}$$

#### 5. Representative Methods for the Solution of the Synthesis Optimization Problem

The design optimization problem can be solved by a number of methods described in the literature (Floudas 1995, Bejan et al. 1996, Stoecker 1989, Rao 1996, Reklaitis et al. 1983, Papalambros and Wilde 2000, Moré and Wright

1993). In this section, representative methods for the solution of the synthesis optimization problem are described in brief, no matter whether they locate the near-optimum solution (classes (a) and (b)) or the optimum one (class (c)) within the constraints and limitations mentioned in Section 3.

### 5.1. The Connectivity matrix method

This method is a direct application of Graph Theory to process design (Bondy and Murty 1976, Linial et al. 1986). It consists of the following steps:

1. Create a logical process scheme. This is a very general task and does not imply the selection or placement of any component. It entails though the selection of the chemical/physical sub-processes that constitute the main process.
2. Construct the Connectivity Matrix (CM) for the logical process scheme. The rows of CM represent fluxes of matter or of energy, while the columns represent "operations" to be performed on these fluxes. A "1" in position  $ij$  signifies that flux  $i$  undergoes transformation  $j$ ; a "0" signals no inter-action of flux  $i$  with sub-process  $j$ . A logical process scheme and its connectivity matrix are shown in *Figure 1* and TABLE I.
3. "Translate" each operation listed in CM into a series of physical transformations and devise one elementary sub-process scheme for each transformation. For example, the operation "boiling" is translated into "pressurized, then fed into a boiler, then superheated, then throttled, then exhausted". Introduce these sub-process schemes into each one of the applicable columns of CM: this corresponds to expanding the matrix by adding several additional columns.
4. Substitute into each transformation in every sub-process the component that performs it. Notice that at this point technical and operational constraints may come into play and limit or deny altogether the feasibility of a certain solution.
5. The resulting matrix is the Connectivity Matrix of the real process P. A proper quantitative simulation of P must now be performed to obtain the optimal set of operational parameters.

It is apparent that this method is a direct translation of the "mental scheme" a Process Engineer applies to a design task, and it is entirely deterministic. Unfortunately, it is also clear that the method is strongly biased by the choices made in points 1 and 3. Choosing a process scheme in fact sets a major structural constraint

on the resulting process configuration, and this step is entirely left to the "experience" of the Designer. Similarly, splitting a process into sub-processes can be done in more than one way, and selecting the one or the other corresponds to biasing the entire procedure. In spite of its limitations, this method has been reported here because it has many similarities with the AI methods that will be discussed later.

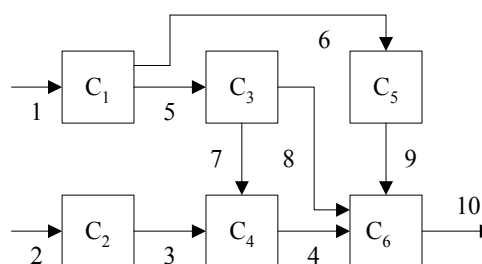


Figure 1. A logical process scheme.

TABLE I. CONNECTIVITY MATRIX OF THE PROCESS IN *FIGURE 1*.

Stream	Component					
	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>	C <sub>5</sub>	C <sub>6</sub>
1	1	0	0	0	0	0
2	0	1	0	0	0	0
3	0	1	0	1	0	0
4	0	0	0	1	0	1
5	1	0	1	0	0	0
6	1	0	0	0	1	0
7	0	0	1	0	0	0
8	0	0	1	0	0	1
9	0	0	0	0	1	1
10	0	0	0	0	0	1

### 5.2. Simulated annealing

Simulated annealing (SA) is a very smart variant of the Matrix Method and, in spite of some limitations that we shall discuss below, is a very reliable Process Synthesizer. Though originally conceived as a multi-variable optimization tool, it was later adapted to function as a structural optimizer (Metropolis et al. 1953). The name is derived from a physical process that will briefly be described before the details of the computational procedure are explained.

When a mass of molten metal is slowly cooled, the temperature distribution inside the body is not uniform: it is usually lower at the external boundaries and hotter inside. Since the thermodynamic energy of the single molecules is proportional to their temperature, organized structures (crystals and grains) begin to appear preferably in the low-temperature areas: their distribution is normally random (in reality, it depends on the presence of "crystallization seeds", but this is irrelevant in our context). If the

cooling is slow enough, the entire body reaches a state of minimum energy, corresponding to the crystalline (and phase) structure in equilibrium at that temperature. If the cooling rate is "too high", there is not sufficient time for the entire body to reach a global minimum energy configuration, and the final structure consists of a certain number of equilibrium crystalline structures (having the minimal energy level compatible with the local temperature) trapped inside of a usually irregular ensemble of "frozen" non-equilibrium entities (crystals and grains whose structures entail higher-than-equilibrium energies or amorphous, frozen liquid). Thus, the final outcome of the process depends on a global external parameter (cooling rate), while the final global energy content may or may not be the global (equilibrium) minimum, depending on the history of the local conditions that were experienced by the various parts of the originally liquid mass upon cooling.

The original idea for simulated annealing was that of constructing an algorithm that could mimic this search for a global optimum by controlling the rate of decrease of a global "energy" parameter (which was called "T", a fictitious temperature) and nesting a sub-optimization for each level of T. The procedure consists of the following steps (Figure 2):

1. Select a Process Superstructure, i.e. a fictitious process Connectivity Matrix (CM) in which all of the components that may be useful in any of the possible sub-processes that lead from input to output are represented. This particular CM has a very high interconnectivity: most components are connected to most others by at least one of the possible fluxes of matter or energy.
2. Establish (define) a global fictitious quantity T that is the functional equivalent of the energy distribution in a solidifying liquid. Assuming we are trying to minimize the objective function, this means that if the system is in state X, with a corresponding value  $f(X)$ , there is a small probability that, for a given T, a different configuration Y, with  $f(Y) > f(X)$  is admissible, i.e. can be reached by the system.
3. Perform a simplified process simulation (if necessary introducing artificial constraints to force some of the most unlikely matches among components) and compute the objective function (usually consisting of a proper combination of performance and cost index).
4. Randomly modify the system interconnection, for instance, by inserting "0" in all entries in a randomly selected column  $k$ :

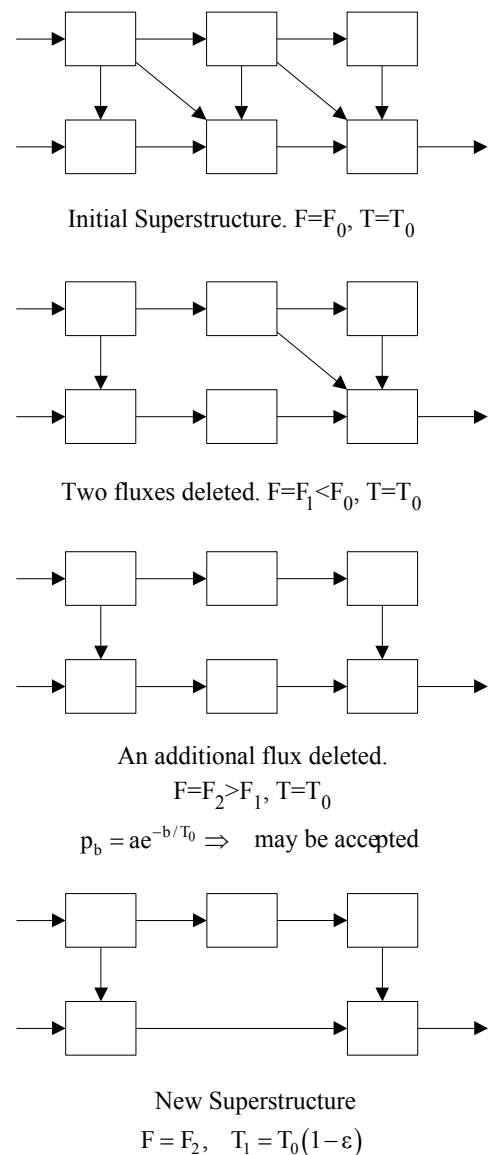


Figure 2. Working principle of simulated annealing.

this corresponds to eliminating component K. Not all "moves" are acceptable: some physical (mass and energy balances) and possibly some configuration constraints apply.

5. Perform a simplified process simulation again and compute the new value of the objective function. If  $f(Y) < f(X)$ , the "new" configuration is accepted. If  $f(Y) > f(X)$ , there is a probability  $p = ae^{-b/T}$  that  $f(Y)$  may still be an acceptable state ( $a$  and  $b$  are arbitrary, case-dependent constants).
6. Decrease T by a pre-assigned amount and repeat steps 4 and 5.
7. Repeat steps 3 to 6 N times: this corresponds in our example to subtracting N components from the initial super-configuration, but other norms for N are ac-

ceptable as well. Record the minimum (or maximum, depending on the case) value of the objective function reached in these  $N$  reduced configurations.

8. Take now as the "new super-configuration" the modified configuration that achieved the lowest (or highest) value of the objective function in the previous  $N$  trials.
9. Repeat steps 3 to 7 until the value of the objective function does not change much from one "new super-configuration" to the next. The last configuration (which is likely to consist of a much lower number of components than the original one) is the sought after "optimal" process structure.

The correct choice of the quantifier  $T$  is crucial in simulated annealing. Unfortunately, its formulation is entirely heuristic, because the analogy between the numerical procedure and the physical annealing process is not perfect. Usually, a dimensionless  $T$  is defined, and its decrease from one level to the next is established a priori by a linear law of the type  $T_{j+1} = T_j(1 - \varepsilon)$  with  $\varepsilon = 1 \div 3\%$ . It is important to remark, though this is rarely mentioned, that the choice of the initial superstructure has a strong influence on the final outcome, SA being in fact strongly biased with respect to its "initial conditions".

### 5.3. Algorithmic approaches

The problem stated by Eqs. (1)-(3) can be solved by direct application of optimization algorithms. Appropriate for this purpose are mixed integer - linear or integer - nonlinear programming algorithms (depending on whether the functions appearing in Eqs. (1)-(3) are linear or nonlinear) and genetic algorithms (Floudas 1995, Goldberg 1989, Gen and Cheng 1997, Chambers et al. 1995). They both operate on a specified superstructure. Usually, integer variables are used to describe the synthesis of the system (e.g., existence or non-existence of components), while real variables correspond to design and operational characteristics of components.

Genetic algorithms have the advantage that they can reveal more than one near-optimal configuration, so the designer may apply additional criteria to select the preferable one. Computationally they are more intense and they, too, can be, if not properly conditioned, rather sensitive to the choice of the initial superstructure ('gene-pool'). It is also possible to combine a genetic algorithm with a linear or nonlinear programming algorithm. The first one is used to effectively reach near-optimal solutions for configuration, design and operation and the second one to determine the exact values of the independent variables at the design and operation levels.

Multilevel optimization and decomposition, which are described below as well as in the aforementioned article, can be used to facilitate the solution.

### 5.4. Targeting methods

The term "supertargeting" also appears in the literature. The ideas originated in the attempt to optimize heat exchanger networks (HEN). One of the targets is the minimum utility cost target and the related problem can be stated as follows:

*Given a heat recovery approach temperature, determine the minimum utility consumption (or utility cost) of a heat exchanger network without prior knowledge of the HEN configuration.*

This is a very important target since it corresponds to the maximum energy recovery that can be attained in a feasible HEN for a fixed heat recovery approach temperature. This target leads to near-optimal solutions (HEN configurations) as long as the energy is the dominant cost item as compared to the investment cost. The key concept that allows for a determination of the minimum utility cost prior to knowing the HEN structure is the *pinch point*. The related concepts and applications are presented in the literature (Linnhoff 1989, Floudas 1995, Frangopoulos 1990, Bejan et al. 1996).

The related methods have been extended in two ways: (i) to include capital and operational expenses other than the cost of utilities, and (ii) to allow application to energy systems that include other components in addition to heat exchangers (e.g., power plants). The whole optimization problem is decomposed into two levels: synthesis of the system directed by thermodynamic targets and then cost minimization. However, this decomposition is not always mathematically correct, leading to inexact solutions of the optimization problem.

### 5.5. The intelligent functional approach

The method is a further development of the Functional Approach described in the literature (Frangopoulos 1983, 1987, 1990). It operates on a superstructure, which is properly analyzed to define the functions of the various components and the related Lagrange multipliers. The values of the Lagrange multipliers, as they are calculated in the procedure, are used to decide on the existence of certain components. Multilevel optimization for the synthesis, design and operation optimization problems is applied. Decomposition can also be applied with respect to subsystems and/or with respect to time, if conditions change with time. A combination of genetic algorithms, nonlinear programming algorithms, and the intel-

ligent functional approach has been successful in reducing the time for solution of the optimization problem.

### 5.6. Decomposition

There are a number of reasons for using decomposition in its various forms to reformulate the optimization problem for energy system synthesis, design, and operation, which in its full complexity is defined as a dynamic, non-linear, mixed-integer programming problem. For example, decomposition can make an intractable, highly complex, highly dynamic problem with a large number of degrees of freedom tractable by breaking the original optimization problem into a set of smaller problems, the solution to which closely approximates the solution of the former. Decomposition may also be warranted when certain company and geographical boundaries (e.g., design teams located far from each other) do not permit solution of the original problem as a single problem.

Three principal types of decomposition exist: *conceptual*, *time*, and *physical*. The first of these decomposes the conceptual aspects of the optimization problem, i.e. synthesis, design, and operation, into two or three levels of optimization (A, B, C, as mentioned in the Introduction). At the operational level, the system is optimized with respect to a set of operational/control variables for a fixed structure (synthesis/design) across an entire load/environmental profile in order to determine optimal system behavior under any (design and off-design) conditions. The results are then integrated over time and introduced at the synthesis level. At this level, a new choice of system configuration (synthesis) is made based on minimizing (or maximizing) the system's objective function with respect to a set of synthesis variables. The results of this optimization are then passed to the design level where for a fixed configuration the system's objective function is minimized (or maximized) with respect to a set of design variables. An iterative procedure is then set up which moves back and forth between the three levels of optimization, terminating once the global optimum for the objective function has been found. This type of decomposition results in a set of nested optimization problems simpler than the original but much more computationally intensive (Olsommer et al. 1999, Frangopoulos 1990).

A variation on this type of decomposition, which avoids this sort of nesting, completely separates the synthesis/design level(s) from the operational level (Munoz and von Spakovsky 2000, 2001a, 2001b). In this approach, the system's synthesis/design is optimized for the most stringent of the load/environmental conditions and a set of optimum and near-optimum feasible

solutions determined for the given synthesis/design point. These feasible solutions are then optimized at all off-design conditions in order to determine the overall optimal solution. This type of decomposition (sometimes referred to as a form of time decomposition in the literature) reduces the computational burden seen with the former approach by assuming that only a limited number of feasible solutions need be optimally evaluated at off-design.

The next type of decomposition is time decomposition, which decomposes the operational optimization problem into a series of quasi-stationary sub-problems each of which correspond to a given time interval. These can be optimized individually with respect to a set of unique operational/control variables and the results summed over all intervals. This form of decomposition complements the others.

In contrast to the two previous types of decomposition, physical decomposition looks at the system itself and breaks it down into a set of units (sub-systems, components, or sub-components), each of which forms a sub-problem within the context of the overall system optimization problem. All such approaches within the literature (e.g., Munoz and von Spakovsky 2000, 2001a, 2001b, von Spakovsky and Evans 1993), can be classified either as a Local-Global Optimization (LGO) or an Iterative Local-Global Optimization (ILGO) approach. In both, it is assumed that a number of disjoint subsets of the set of synthesis/design variables (one set for each unit and one, if needed, at the system level) can be established. Each set at the unit-level is used to optimize its respective sub-problem while the system-level set is used to optimize the overall problem at the system-level. In LGO, this results in a nested set of optimizations of unit-level problems within an overall system-level problem.

A conceptual depiction of this approach is seen in *Figure 3* where, for example, at the unit-level the local objective  $C_1$  is optimized (see the highly non-linear surface on the far right in *Figure 3*) with respect to its disjoint sub-set of variables  $\mathbf{w}_1, \mathbf{z}_1$ . This optimization occurs for fixed values ( $\xi, \psi$ ) of the system-level set of variables or coupling functions  $u_{ij}$ . The other units are likewise optimized locally and this process is repeated many times for different values of the coupling functions. The final result of this process is a set of unit-level optimum response surfaces (ORSs), the combination of which results in the system-level ORS seen in *Figure 3*. The system-level optimum is then found at the lowest point (if a minimization) on this surface (*Figure 3*).

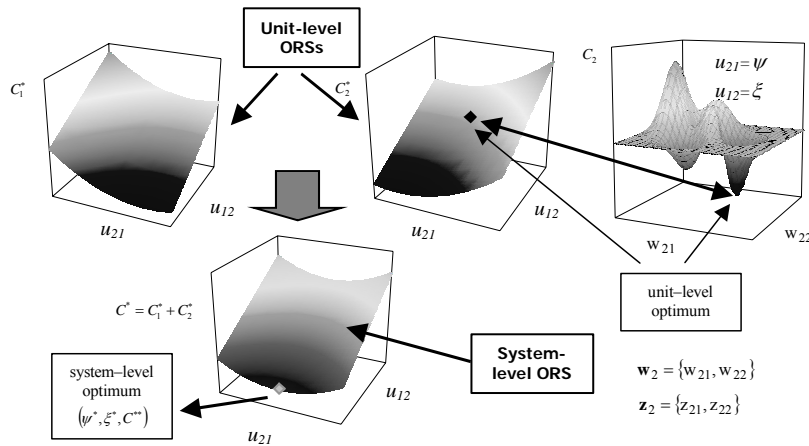


Figure 3. Local (unit-level) and global (system-level) optimizations for LGO and ILGO

Of course, as with the other decomposition approaches, the principle disadvantage of LGO is that it is very computationally intensive. To circumvent this, ILGO instead of LGO may be applied since the former avoids the need for creating any of the ORSs and avoids as well the nesting inherent in the other decomposition approaches. ILGO accomplishes the former by using derivative information in the form of what are called *shadow prices* (derivatives of the optimal value of a function with respect to certain variables) to intelligently move along the system-level ORS towards the system-level optimum, and it accomplishes the latter by incorporating system-level information directly into the unit-level objectives through the use of *shadow prices*

### 5.7. Artificial Intelligence and Expert Systems techniques

In the preceding, it is tacitly assumed that *all* process design calculations can be carried out by properly implemented automated routines. Process design is a highly labor intensive and highly interdisciplinary task and is, therefore, by necessity performed by a team of specialists: as a consequence, it is also very expensive in monetary terms, and there is a strong incentive to reduce this labor intensity (measured in man-hours). The only task that has as of yet not been fully automated is the *conceptual* one: the choice of the type and of the characteristics of the process itself. This automation can be implemented by a direct application of the very powerful Artificial Intelligence (AI) techniques, whose specific task is to allow the codification of procedures that somehow mimic the thinking patterns of the human mind. Currently, only a subset of these techniques, called Expert Systems (ES), have been successfully applied to energy systems. ESs can be used to reproduce the engineer's decisional path that proceeds from the design data and constraints to possible process configurations.

Expert Systems are based on *relational languages* that use the symbolism of formal propositional logic. They draw inferences from a number of *facts* stored in a particular database, properly called a *knowledge base*. These facts can be design data, design rules, physical or logical constraints, etc. Each ES manipulates this knowledge in its own way, according to a logical procedure contained in its *inference engine*. Space limitations do not allow a detailed presentation of AI and ES techniques, but the interested reader can find information in the literature (Sciubba and Melli 1998, Sriram 1997, Green 1992).

### 6. Closure

As one goes from operation optimization to design and synthesis optimization of energy systems, the problem becomes much more difficult not only from a computational but also from a methodological point of view. Several methods have been developed, which have been shown to be successful at least for particular classes of problems, even when the number of degrees of freedom is large and the models involved highly nonlinear and complex. However, the effort to develop even more capable and more generally applicable methods continues.

### References

- Bausa, J., and Tsatsaronis, G., 2001, "Dynamic Optimization of Startup and Load-increasing Processes in Power Plants – Part I: Method, Part II: Application," *ASME Journal of Engineering for Gas Turbines and Power*, Vol. 123, pp. 246-254.
- Bejan, A., Tsatsaronis, G., and Moran, M., 1996, *Thermal Design and Optimization*, John Wiley & Sons, New York.
- Bondy, J. A., and Murty, U.S.R., 1976, *Graph Theory with Applications*, Elsevier.



- Chambers, L., ed., 1995, *Practical Handbook of Genetic Algorithms*. Vol. I: Applications, Vol. II: New Frontiers, CRC Press, New York.
- Floudas, C. A., 1995, *Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications*, Oxford University Press, New York.
- Frangopoulos, C. A., 1983, "Thermoeconomic Functional Analysis: A Method for Optimal Design or Improvement of Complex Thermal Systems," Ph.D. Thesis, Georgia Institute of Technology, Atlanta, Ga.
- Frangopoulos, C. A., 1987, "Thermoeconomic Functional Analysis and Optimization," *Energy*, Vol. 12, No. 7, 563-571.
- Frangopoulos, C. A., 1990, "Intelligent Functional Approach: a Method for Analysis and Optimal Synthesis-Design-Operation of Complex Systems," *A Future for Energy*, S. S. Stecco and M. J. Moran, eds., Florence World Energy Research Symposium, Florence, Italy, May 28-June 1, pp. 805-815, Pergamon Press, Oxford.
- Frangopoulos, C. A., Lygeros, A. I., Markou, C. T. and Kaloritis P., 1996, "Thermo-economic Operation Optimization of the Hellenic Aspropyrgos Refinery Combined-cycle Cogeneration System," *Applied Thermal Engineering*, Vol. 16 No. 12, pp. 949-958.
- Gen, M., and Cheng, R., 1997, *Genetic Algorithms and Engineering Design*, J. Wiley and Sons, New York.
- Goldberg, D. E., 1989, *Genetic Algorithms in Search, Optimization and Machine Learning*, Addison-Wesley Publishing Co., Inc., Reading, Massachusetts.
- Green, M., ed., 1992, *Knowledge Aided Design*, Academic Press.
- Kott, A. S., May, J. H. and Hwang, C. C., 1989, "An Autonomous Artificial Designer of Thermal Energy Systems: Part 1 – Theoretical Considerations, Part 2 – Solution Algorithm," *ASME Journal of Engineering for Gas Turbines and Power*, Vol. 111, pp. 728-739.
- Linial, N., Lovasz, L., and Widgerson, A., 1986, "A Geometric Interpretation of Graph Connectivity and its Algorithmic Applications," *27th Symposium on Foundations of Computer Science*, pp. 39-48.
- Linnhoff, B., et al., 1982, *A User Guide on Process Integration for the Efficient Use of Energy*, Institution of Chemical Engineers, Rugby, Warks, England.
- Linnhoff, B., 1989, "Pinch Technology for the Synthesis of Heat and Power Systems," *J. of Energy Resources Technology*, Vol. 111, pp. 137-148.
- Metropolis, N., Rosenbluth, A., Teller, A., and Teller, E., 1953, "Equation of State Calculations by Fast Computing Machines," *J. Chem. Phys.*, Vol. 21, No. 6, pp. 1087-92.
- Moré, J. J., and Wright, S. J., 1993, *Optimization Software Guide*, Society of Industrial and Applied Mathematics, Philadelphia, Pennsylvania.
- Munoz, J. R., and von Spakovsky, M. R., 2000, "The Use of Decomposition for the Large Scale Thermoeconomic Synthesis / Design Optimization of Highly Coupled, Highly Dynamic Energy Systems – Theory and Application," *International Mechanical Engineering Congress and Exposition, IMECE 2000*, ASME, AES-Vol. 40, pp. 213-249.
- Munoz, J. R., and von Spakovsky M. R., 2001a, "A Decomposition Approach for the Large Scale Synthesis / Design Optimization of Highly Coupled, Highly Dynamic Energy Systems," *International Journal of Applied Thermodynamics*, Vol. 4 No. 1, pp. 19-33.
- Munoz, J. R., and von Spakovsky M. R., 2001b, "The Application of Decomposition to the Large Scale Synthesis / Design Optimization of Aircraft Energy Systems," *International Journal of Applied Thermodynamics*, Vol. 4, No. 2, pp. 61-76.
- Olsson, B., von Spakovsky, M. R., and Favrat, D., 1999, "An Approach for Time-dependent Thermoeconomic Modeling and Optimization of Energy System Synthesis, Design and Operation: Part I – Methodology and Results, Part II – Reliability and Availability," *International Journal of Applied Thermodynamics*, Vol. 2 No. 3, 1999, pp. 97-114, and Vol. 2 No. 4, pp. 177-186.
- Papalambros, P. Y., and Wilde, J., 2000, *Principles of Optimal Design – Modeling and Computation*, Cambridge University Press, Cambridge, U.K.
- Rao, S. S., 1996, *Engineering Optimization: Theory and Practice*, 3<sup>rd</sup> ed., J. Wiley & Sons, Inc., New York.
- Reklaitis, G. V., Ravindran, A., and Ragsdell, K. M., 1983, *Engineering Optimization – Methods and Applications*, J. Wiley & Sons, New York.
- Sciubba, E., 1998, "Toward Automatic Process Simulators: Part I – Modular Numerical Procedures, Part II – An Expert System for Process Synthesis," *ASME Journal of Engineering for Gas Turbines and Power* Vol. 120, pp. 1-16.
- Sciubba, E., and Melli, R., 1998, *Artificial Intelligence in Thermal Systems Design: Concepts and Applications*, Nova Science Publishers, Inc., Commack, New York.

Sriram, R. D., 1997, *Intelligent Systems for Engineering*, Springer Verlag.

Stoecker, W. F., 1989, *Design of Thermal Systems*, McGraw-Hill, Inc., New York.

von Spakovsky, M. R., and Evans, R. B., 1993, "Engineering Functional Analysis – Parts I, II," *ASME Journal of Energy Sources Technology*, Vol. 115, pp. 86-99.