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A Decomposition Approach for the Large Scale Synthesis/Design Optimization of Highly Coupled, Highly Dynamic Energy Systems

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Abstract

A general methodology for the decomposed optimization of highly coupled, highly dynamic energy systems is presented. The approach is based on the physical division of the system into units (sub-systems, components or disciplines) subject to functions describing the energy, cost and other couplings between them. Two versions of the approach are proposed. The first approach is called the Local-Global Optimization (LGO) Approach. LGO requires unit optimizations to be carried out with respect to purely local decision variables for various combinations of the functions that connect the units. The results are used to create an Optimum Response Surface (ORS) for the entire problem. The ORS is then searched by a system-level optimizer to find the values of the coupling functions that lead to an optimum system-level solution. The second approach proposed is an iterative version of LGO (ILGO). In this case, the ORS is closely approximated using a linear Taylor series expansion. The partial derivatives resulting from such an approximation are seen to correspond to the shadow prices (or marginal costs) typically used in the thermoeconomic literature. ILGO effectively and significantly reduces the number of unit optimizations required. The properties used to describe the coupling functions play a critical role in the convergence of ILGO to a global system-level optimum. A discussion of this and its implication for the choice of First or Second-Law based quantities for the optimization of systems is given.

Key words: decomposition, optimization, synthesis, thermal design, thermoeconomics

1. Introduction

The integrated synthesis/design of highly integrated energy systems with variable loads and/or environmental conditions is a research area of great interest. In this paper, *decomposition* is used as a tool for overcoming the mathematical, cultural, and software difficulties that can occur if the design problem is formulated as a single problem for the system as a whole. *Decomposition* is seen as a tool that not only permits the solution of the overall synthesis/design problem by dividing it into smaller sub-problems but facilitates the difficult task of sub-system integration. The problem of integration is not only that the synthesis/design of the different subsystems usually present in complex systems is accomplished by teams generally in different areas of expertise each using tools possibly incompatible with those used in other areas but also that these teams encompass a wide variety of engineering disciplines. In addition, the synthesis/design of the different sub-systems may, in many cases, be done at different stages and at times crossing company lines. Furthermore, it is not uncommon

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to have design teams that are not located entirely at one facility that, added to cultural differences, complicates the task at hand even further. The methods presented here are seen to match and enhance existing design practices and are in tune with the current need for concurrent, collaborative environments that make use of multiprocessing as well as parallel and internet capabilities.

To demonstrate the generality of the decomposition methods presented here, the systems considered are quite general and, thus, may represent, for example, stationary or aircraft/aerospace applications. It is assumed throughout this paper that any system modeling may require a high level of detail (and is, therefore, expensive to simulate and optimize) and may involve large numbers of continuous and discrete variables. The synthesis/design problem is set up in a general way so that streams and feedbacks (i.e. couplings) between units[1] may be represented by energy (or exergy) or by any other relevant quantity that may, for example, facilitate the interface with non-energy systems. This contrasts with the El-Sayed and Evans (1970) formalism and other thermoeconomic formulations (e.g., Frangopoulos, 1983; Tsatsaronis, 1985; von Spakovsky, 1986; Valero et al., 1986; Benelmir, 1990; etc.), which were developed under the assumption that the properties of the energy system being considered are best expressed in terms of exergy. These formulations used exergy due to the belief that cost accounting is more rationally achieved with the use of exergy. For analysis purposes, this is indeed the case! However, even the most enthusiastic proponents of Second Law analysis know that exergy is not an essential requirement for optimization although in certain cases there may be an associated advantage to its use[2]. In this paper, the final choice of quantity (or quantities) used to represent streams and feedbacks (i.e. couplings) is based on ensuring that the shadow prices (or marginal costs)[3] associated with these quantities exhibit certain desirable properties (e.g., aid in decomposition and subsystem integration). Whether the choice is exergy or energy or something else depends on this and certain practical considerations such as the details of the simulations tools available, the level of expertise present, the number of different disciplines required, etc.

2. The Synthesis and Design Optimization of Dynamic Energy Systems

Consider a general non-hierarchical[4] system[5] composed of three units (sub-systems, components, disciplines, or simply black-boxes) as shown in *Figure 1*. Three is considered a small enough number to understand the features of the methods yet large enough to reveal patterns and facilitate the use of compact mathematics. The results presented in this paper can be routinely extended to systems with more than three units. In *Figure 1*, the functions u_{ij} are called coupling, compatibility, linking or connecting functions. The coupling functions can also be considered intermediate forward and backward feedback functions. Each unit has its own vector of decision variables $\vec{x}_i$ and a local contribution, f_i, to the overall objective function, f. The objective function is often called the cost function. Although not all design problems have this feature, it is very typical in energy systems. In this kind of system, a unit's contribution to the overall objective function takes the form:

$$f_i = k_i R_i + Z_i \qquad (1)$$

where the functions R_i $(i = 1,..., m)$ represent the external resources (e.g., fuel) used to perform the required tasks. These tasks are assumed known. The functions Z_i are related to the physical dimensions and material and technology choices for the unit and can, therefore, be given in terms of mass, area, volume and/or capital cost. The Z_i will, thus, be called the capital functions. The constant k_i is an appropriate conversion factor.

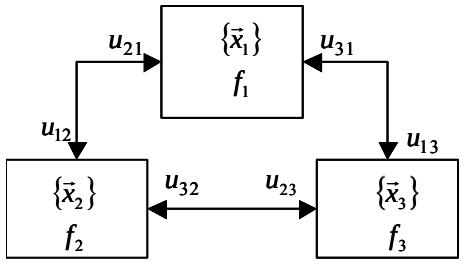

Figure 1. A coupled non-hierarchical system.

One of the features of dynamic energy systems is that the amount of external resources may vary in time. Likewise, under certain

[1] Units in this context refer to either subsystems or components.

[2] For example, it may be used as the basis of a search engine for finding the global optimum; or in certain cases, it may enhance *decomposition* itself.

[3] "Marginal cost" and "shadow price" are not synonymous but are nonetheless used interchangeably here, since under the conditions specified in the paper, the "shadow price" is the marginal cost associated with marginal changes in a unit or local objective's optimum value with respect to marginal changes in the value of an associated coupling function.

[4] A non-hierarchical system is one in which each decision, even a localized decision, influences the rest of the system.

[5] In order to be as general as possible, the term "system" is used here to refer to any engineering system whether energy based or not.

circumstances, the capital functions may take different values over time. One such circumstance is when the capital function represents costs that may be influenced by operating conditions (e.g., maintenance costs). Another feature of energy systems is that the coupling functions u_{ij} may be interpreted as intermediate products of unit i, which become intermediate resources for unit j. In some cases, the coupling functions can be considered as attributes of j that are passed back to i, i.e. they effectively act as intermediate feedback functions.

Time variations in the local objective functions are handled by defining the independent synthesis/design and operational variables $\vec{x}_i$ and $\vec{y}_{it}$, respectively, for each unit. The synthesis/design variables, $\vec{x}_i$, typically correspond to geometric parameters (physical unit dimensions), design flow rates, design pressure ratios, as well as discrete (e.g., material or technology choices) or binary (e.g., unit existence or nonexistence) parameters. By definition synthesis/design variables remain constant in time. Operational variables, $\vec{y}_{it}$, are parameters which can be controlled over time so that off-design operation is optimal. Operational variables can be continuous variables (flow rates, valve settings) or binary variables (e.g., units on or off).

Given the dynamic nature of the problem, it is often convenient to work with objective functions in rate form. The functional relationships for the local objective functions at an instant of time *t* are then given by:

$$\begin{aligned}\dot{R}_1 &= \dot{R}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(u_{12}, u_{13}, u_{21}, u_{31}\right)_t\right)\\ \dot{R}_2 &= \dot{R}_2\left(\vec{x}_2, \vec{y}_{2t}, \left(u_{21}, u_{23}, u_{12}, u_{32}\right)_t\right)\\ \dot{R}_3 &= \dot{R}_3\left(\vec{x}_3, \vec{y}_{3t}, \left(u_{13}, u_{31}, u_{32}, u_{23}\right)_t\right)\end{aligned} \tag{2}$$

$$\begin{aligned}\dot{Z}_1 &= \dot{Z}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(u_{12}, u_{13}, u_{21}, u_{31}\right)_t\right)\\ \dot{Z}_2 &= \dot{Z}_2\left(\vec{x}_2, \vec{y}_{2t}, \left(u_{21}, u_{23}, u_{12}, u_{32}\right)_t\right)\\ \dot{Z}_3 &= \dot{Z}_3\left(\vec{x}_3, \vec{y}_{3t}, \left(u_{13}, u_{31}, u_{32}, u_{23}\right)_t\right)\end{aligned} \tag{3}$$

and

$$\begin{aligned}\dot{f}_1 &= \dot{f}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(u_{12}, u_{13}, u_{21}, u_{31}\right)_t\right)\\ \dot{f}_2 &= \dot{f}_2\left(\vec{x}_2, \vec{y}_{2t}, \left(u_{21}, u_{23}, u_{12}, u_{32}\right)_t\right)\\ \dot{f}_3 &= \dot{f}_3\left(\vec{x}_3, \vec{y}_{3t}, \left(u_{13}, u_{31}, u_{32}, u_{23}\right)_t\right)\end{aligned} \tag{4}$$

At an instant of time *t*, the coupling functions are in general given by

$$u_{ij_t} = u_{ij}(\vec{x}_i, \vec{x}_j, \vec{y}_{it}, \vec{y}_{j_t}) \tag{5}$$

With this in mind and after choosing the independent variables, the system-level synthesis/design problem is formulated as:

$$\text{minimize } f = \int_{\text{time}} \left(\sum_{i=1}^{3} \dot{f}_{it} \right) dt \tag{7}$$

$$\text{w.r.t. } \vec{X} = \{\vec{x}_1, \vec{x}_2, \vec{x}_3\};\quad \vec{Y} = \left\{\vec{Y}_t\right\} = \left\{\vec{y}_{1t}, \vec{y}_{2t}, \vec{y}_{3t}\right\}$$

subject to:

$$\vec{H} = \left\{\vec{H}_t\right\} = \begin{Bmatrix} \vec{h}_{1t} \\ \vec{h}_{2t} \\ \vec{h}_{3t} \end{Bmatrix} = \vec{0} \tag{6.1}$$

$$\vec{\Gamma} = \left\{\vec{G}_t\right\} = \begin{Bmatrix} \vec{g}_{1t} \\ \vec{g}_{2t} \\ \vec{g}_{3t} \end{Bmatrix} \le \vec{0} \tag{6.2}$$

where:

$$\dot{f}_i = k_i \dot{R}_i + \dot{Z}_i \tag{6.3}$$

The vectors of equality and inequality constraints at various instants of time, $\vec{H}_t$ and $\vec{G}_t$, represent the thermodynamic, physical and cost models (i.e. the analysis system of equations) and the restrictions imposed on the synthesis/design. One such restriction is the desired product for each of the units. Thus, the n_{th} element of any vector of equality constraints $\vec{h}_i$ at any instant t is given by:

$$h_{i,n_t} = \dot{P}_{it} - \dot{P}^{o}_{it} \tag{6.4}$$

where $\dot{P}_{it}$ is the actual product rate and $\dot{P}^{o}_{it}$ the rate of product required from unit i.

In most cases it is advisable to discretize the time integral by taking time segments (independent of each other or not[6]) over the entire load and/or range of environmental conditions. The number of these segments depends on the nature of the load and the level of detail desired. A discretized version of Eq. (6) can be written as:

$$\text{minimize } f = \sum_{t=1}^{\tau} \left(\sum_{i=1}^{3} \dot{f}_i \right) \Delta t_t \tag{7}$$

$$\text{w.r.t. } \vec{X} = \{\vec{x}_1, \vec{x}_2, \vec{x}_3\};\ \vec{Y} = \left\{\vec{Y}_t\right\} = \left\{\vec{y}_{1t}, \vec{y}_{2t}, \vec{y}_{3t}\right\}$$

$$t = 1,..., \delta,..., \tau$$

subject to:

[6] A problem with dependent time segments is one for which transient effects are important.

$$\vec{H} = \left\{\vec{H}_t\right\} = \begin{Bmatrix} \vec{h}_{1t} \\ \vec{h}_{2t} \\ \vec{h}_{3t} \end{Bmatrix} = \vec{0} \quad t = 1,..., \delta,..., \tau \qquad (7.1)$$

$$\vec{\Gamma} = \left\{\vec{G}_t\right\} = \begin{Bmatrix} \vec{g}_{1t} \\ \vec{g}_{2t} \\ \vec{g}_{3t} \end{Bmatrix} \le \vec{0} \quad t = 1,..., \delta,..., \tau \qquad (7.2)$$

Here the subscript t refers to the τ different segments into which the load/environmental conditions have been divided. Note that Eq. (7) allows time segments of different durations.

Now, assume that the sizes of the synthesis/design and operational variable vectors are d and o, respectively. The total number of variables is, therefore, $d+o\tau$. For complex, highly dynamic energy systems, which may require high levels of detail and/or have large numbers of units, the total combined number of variables, discrete and continuous, may grow very large. In addition, the fact that the response of energy system components and subsystems is typically highly nonlinear and the nature of the design space non-contiguous (due to the presence of discrete/binary variables) makes the problem very expensive computationally and in some cases, even impossible to be solved with existing optimization algorithms. In fact, the resulting mixed-integer, non-linear programming (MINLP) problem has a known solution only under very special, restricted conditions (Floudas, 1995; Bruno et al., 1998).

The alternatives normally considered are to reduce the number of independent variables either by varying only a few synthesis/design variables at a time (trade-off analysis), considering a severely limited number of synthesis/design variables while accounting for only one of the operating conditions (one-point synthesis/design), and/or linearizing the problem in order to transform it into a mixed integer linear programming (MILP) or linear programming (LP) problem. These alternatives can be avoided through the use of *decomposition* so that the solution to the original problem does not compromise the quality of the final synthesis/ design.

However, the purpose of *decomposition* is not just to decrease the size of the synthesis/design problem. An equally important reason is to facilitate the difficult task of sub-system and, in some cases, discipline integration. In many existing industrial design processes, the synthesis/design of units is carried out by different groups and oftentimes different departments within a company or even different companies. The different design philosophies, tools and procedures are in many cases not compatible with each other, making the solution of the entire problem as a single block simply impractical. These difficulties are only worsened by the fact that the synthesis/design of the different units is done at different times.

Therefore, in many practical settings, *decomposition* is an absolute necessity. In this work, two types of decomposition are considered. The first is *time decomposition* and the second *physical* (i.e. unit) *decomposition*. Physical or unit decomposition uses the Local Global (LGO) and Iterative Local Global (ILGO) optimization methods developed by Muñoz and von Spakovsky (2000 a, b, c).

2.1 Time decomposition

Time decomposition exploits the fundamental differences that exist between the design and operational variables to create a set of hierarchical problems each with a lower dimensionality than the overall system-level problem. Different types of time decomposition can be defined.

The most common time decomposition (e.g., Frangopoulos (1989), Olsommer, et al (1999a,b)) consists of initially selecting values for the synthesis/design variables ($\vec{X}$) and then searching for the optimum values of the operational decision variables ($\vec{Y}_t$). The latter low-level optimization can be done taking all of the time segments into which the load/environmental conditions have been divided and using them in a single problem. If the number of operational decision variables (e.g., the size of the vector $\vec{Y}$) and/or the number of time segments is large, it may be advisable to define a set of τ optimization problems, one for each of the time segments (each with respect to the instantaneous operational variable vectors ($\vec{Y}_t$)). Once the lower-level problems are solved, the optimum values of the objective functions corresponding to the given synthesis/design variables are sent back to a high-level optimizer for analysis. The high-level optimizer is in charge of finding the optimum values for the synthesis/design variables ($\vec{X}$).

The so-called nested time decomposition described above, effectively reduces the size of the overall problem from $d+o\tau$ variables by solving two problems of size d and $o\tau$ or a combination of one problem of size d and τ problems of size o. The main disadvantages of nested time decomposition approaches are:

- the very large expense of the nested optimizations that result from applying either approach (i.e. all the time segments as a

single problem or each time segment as an individual problem).
- the size of the sub-problems may still be too large even with time decomposition.
- other forms of decomposition, e.g., physical decomposition, are difficult to implement at the synthesis/design level.
- it is likely that a number of combinations of the synthesis/design variables $\vec{X}$ when used in the lower-level problem(s) (to find the optimum $\vec{Y}_t$ *values*) will not lead to feasible solutions.

Other than the third disadvantage above, all of these drawbacks are alleviated somewhat by the fact that both approaches are easily parallelized in various ways. Thus, for example, multiple processors may simultaneously handle different combinations of the synthesis/design variables along with the optimizations with respect to the operational variables. Another possibility is to have multiple processors execute the τ optimizations of the different time segments.

In order to get around the third disadvantage listed above and at the same time minimize the others as well, the type of time decomposition proposed and used in this work is <u>not</u> nested and consists of selecting one time segment, say segment δ, which has the most demanding[7] load requirements and/or environmental conditions[8], as the synthesis/design point[9]. The system is then synthesized/designed for this point by solving the restricted problem:

$$\text{minimize } f_\delta = \left[\left(\sum_{i=1}^{3} \dot{f}_i\right)\Delta t\right]_\delta \tag{8}$$

$$\text{w.r.t. } \vec{X} = \{\vec{x}_1, \vec{x}_2, \vec{x}_3\};\ \vec{Y} = \{\vec{Y}_\delta\} = \{\vec{y}_{1\delta}, \vec{y}_{2\delta}, \vec{y}_{3\delta}\}$$

subject to:

$$\vec{H}_\delta = \begin{Bmatrix} \vec{h}_{1\delta} \\ \vec{h}_{2\delta} \\ \vec{h}_{3\delta} \end{Bmatrix} = \vec{0} \tag{8.1}$$

$$\vec{G}_\delta = \begin{Bmatrix} \vec{g}_{1\delta} \\ \vec{g}_{2\delta} \\ \vec{g}_{3\delta} \end{Bmatrix} \le \vec{0} \tag{8.2}$$

where Δt is the length of time considered for all time segments (i.e. $\Delta t = \sum_{t=1}^{\tau} \Delta t_t$). The subscript δ refers to the segment chosen for the "synthesis/design" point of the system.

The result obtained from solving Eq. (8) for a single synthesis/design is a set of feasible solutions[10] (one optimal with respect to Eq. (8) and others not) that satisfies the constraints given by Eq. (8.2). These solutions have a corresponding set of vectors $\vec{X}_\delta$ and $\vec{Y}_\delta$. The most promising of these feasible solutions (each having decision variables $\vec{X}_\delta^{fp}$ and $\vec{Y}_\delta^{fp}$, and corresponding objective function value f_δ^{fp}) are then used to minimize the total cost over the entire load/environmental profile for each of these feasible solutions, i.e.:

minimize:

$$f = \left[\left(\sum_{i=1}^{3} \dot{f}_i^{fp}\right)\Delta t\right]_\delta + \sum_{t=1}^{\tau-1}\left(\sum_{i=1}^{3} \dot{f}_i\right)\Delta t_t \tag{9}$$

$$\text{w.r.t. } \vec{Y} = \{\vec{Y}_t\} = \{\vec{y}_{1t}, \vec{y}_{2t}, \vec{y}_{3t}\}$$
$$t = 1,\ldots,\delta-1,\delta+1,\ldots,\tau$$

subject to:

$$\vec{H} = \{\vec{H}_t\} = \begin{Bmatrix} \vec{h}_{1t} \\ \vec{h}_{2t} \\ \vec{h}_{3t} \end{Bmatrix} = \vec{0};\quad t = 1,\ldots,\delta-1,\delta+1,\ldots,\tau$$
$$\vec{\Gamma} = \{\vec{G}_t\} = \begin{Bmatrix} \vec{g}_{1t} \\ \vec{g}_{2t} \\ \vec{g}_{3t} \end{Bmatrix} \le \vec{0};\quad t = 1,\ldots,\delta-1,\delta+1,\ldots,\tau \tag{9.1}$$

and $\vec{X} - \vec{X}_\delta^{fp} = \vec{0}$ (9.2)

This type of decomposition uses the implicit assumption that some synthesis/design variables $\vec{X}$ are likely to lead to an optimum solution when the period of operation is included. The first term on the right of Eq. (9) is known from solutions to Eq. (8). It is furthermore assumed that the best solutions for the reference (synthesis/design) point found from problem (8) are not necessarily the best when integrated over

[7] The most demanding segment could be the one that uses the greatest amount of external resources and/or poses the greatest challenges in terms of satisfying the system analyzer equations including the external demand for the system's products.

[8] Actually, more than one segment could be chosen especially if *a priori* it were not clear which segment is the most demanding or if two or more segments are relatively close in significance. Of course, each additional segment complicates the process and too many defeat the purpose of this type of non-nested time decomposition all together.

[9] A single reference condition is normally called the synthesis/design point. In this context, such a designation is somewhat misleading since one is trying to obtain the synthesis/design that minimizes the cost over the entire period of operation.

[10] This presupposes a means for generating these feasible solutions, which can be done with a heuristic approach such as a genetic algorithm or conventional gradient-based method.

the various off-design conditions. To this end, as indicated by constraint (9.2), the values of the synthesis/design variables are set equal to the various synthesis/design variable values associated with the promising feasible solutions obtained from solving problem (8).

The type of time decomposition proposed effectively transforms a problem with d+oτ variables into two problems (one of synthesis/design and the other of operation), the latter of which can be divided further into τ^{-1} problems since one can define (τ-1) off-design optimization problems (implemented in parallel) with respect to the instantaneous operational decision variables (Y_t). The synthesis/design problem will, thus, have d+o decision variables while each of the operational or off-design problems will have *o* decision variables. The reduced number of variables for the decomposed problem, however, comes at the expense of possibly having to carry out the optimization problem given by problem (9) for several possible feasible (but promising) solutions found by solving the reduced problem given by problem (8). An obvious advantage over the nested time decomposition approaches described earlier is that no time is spent on solutions that i) are infeasible or ii) do not meet the most stringent demand and operating conditions.

Even with time decomposition, the solution of the synthesis/design problem (problem (8)) may be problematic if the number of variables (d+o) is still very large. In this case, time decomposition reduces the number of variables for each decomposed operational problem but does not completely facilitate the solution of the overall problem. Thus, an additional decomposition is necessary.

2.2 Physical (unit) decomposition in energy system synthesis and design

Depending on the size of the problem (number of units, number of inputs/outputs of each unit, number and nature of the independent variables), any of the approaches developed by Muñoz and von Spakovsky (2000 b, c) can be considered for solving the overall problem using *physical decomposition*. The first is the Local-Global Optimization (LGO) approach and the second the Iterative Local-Global Optimization (ILGO) approach applied to energy systems. Both decomposition approaches use certain desirable properties of the shadow prices (marginal costs) associated with the energy and cost flow couplings between units to facilitate the optimization and the convergence of the process. In order to apply any of these methods, let us consider the three-unit energy system of *Figure 1*. The synthesis/design problem for this system is to:

minimize:

$$f = \sum_{t=1}^{\tau} \begin{bmatrix} \dot{f}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(u_{21}, u_{31}, u_{12}, u_{13}\right)_t\right)\Delta t_t \\ + \dot{f}_2\left(\vec{x}_2, \vec{y}_{2t}, \left(u_{12}, u_{32}, u_{21}, u_{23}\right)_t\right)\Delta t_t \\ + \dot{f}_3\left(\vec{x}_3, \vec{y}_{3t}, \left(u_{13}, u_{23}, u_{31}, u_{32}\right)_t\right)\Delta t_t \end{bmatrix} \quad (10)$$

$$\text{w.r.t. } \vec{X} = \{\vec{x}_1, \vec{x}_2, \vec{x}_3\};\ \vec{Y} = \{\vec{Y}_t\} = \{\vec{y}_{1t}, \vec{y}_{2t}, \vec{y}_{3t}\}$$
$$t = 1,..., \delta,..., \tau$$

subject to the primary constraints:

$$H\vec{H} = \{\vec{H}_t\} = \begin{Bmatrix} \vec{h}_{1t} \\ \vec{h}_{2t} \\ \vec{h}_{3t} \end{Bmatrix} = \vec{0} \quad t = 1,..., \delta,..., \tau \quad (10.1)$$

$$\vec{\Gamma} = \{\vec{G}_t\} = \begin{Bmatrix} \vec{g}_{1t} \\ \vec{g}_{2t} \\ \vec{g}_{3t} \end{Bmatrix} \le \vec{0} \quad t = 1,..., \delta,..., \tau \quad (10.2)$$

2.3 Local-global optimization (LGO) approach for energy systems

In the Local-Global Optimization (LGO) approach, the units (disciplines) are decomposed and the resulting problems are solved for different values of the unit couplings. The optimum results are used by a system-level optimization problem, which optimizes with respect to the coupling functions (Muñoz and von Spakovsky, 2000 a, b, c).

In order to apply the LGO approach to the design/optimization of the energy system of *Figure 1*, it is assumed that the coupling functions u_{ij}, i.e. the intermediate feedbacks, are kept at a constant value ξ_{ij} at each instant of time, i.e.:

$$\{u_{ij}\}_t = \{\xi_{ij}\}_t \quad t = 1,..., \delta,..., \tau \quad (11)$$

From close inspection of problem (10) and the functional relationships for the coupling functions given by Eq. (5), it is clear that the decision variable vectors $\vec{x}_i$ and $\vec{y}_{it}$ are strictly local and that the u_{ij} are the only link between unit i and the rest of the system. The fact that the u_{ij} are kept fixed allows one to define a local optimization problem for unit 1 and a different one for units 2 and 3 combined or two different ones for units 2 and 3 as separate entities[11]. For example, as mentioned above, the following local (unit) synthesis/design problem for unit 1 could be defined:

[11] Further decompositions are, of course, also possible for each of the units.

minimize:

$$f_1 = \sum_{t=1}^{\tau} \dot{f}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(\xi_{21}, \xi_{31}, \xi_{12}, \xi_{13}\right)_t\right)\Delta t_t \qquad (12)$$

w.r.t. $\vec{x}_1$, $\vec{y}_{1t}$ $\quad t = 1,...,\delta,...,\tau$

subject to:

$$\vec{h}_{1t} = \vec{0} \quad t = 1,...,\delta,...,\tau \qquad (12.1)$$

$$\vec{g}_{1t} \le \vec{0} \quad t = 1,...,\delta,...,\tau \qquad (12.2)$$

The requirement imposed by Eq. (11) on the values for the coupling functions may be overly restrictive, particularly if the values of the coupling functions at different instants are dependent on each other. In such cases, it is advisable to use the time decomposition scheme presented above and solve the problem in two sequential steps. In the first step, problem (12) and the corresponding ones for units 2 and 3 are solved at one load/environmental condition, δ, judged to be the most critical so that it becomes the synthesis/design condition. The most promising solutions from these problems are then used to minimize the sum of the local (unit) objective functions at all the other off-design conditions.

The solutions obtained from solving problem (12) and similar problems defined for units 2 and 3 are the restricted local (unit-based) optimum cost rates at different times $\left\{\dot{f}_{i\,t}^{*}\right\}$ and their corresponding restricted total optimum values f_i^* as well as the optimum operational decision variables at all instants of time $\left\{\vec{y}_{i\,t}^{*}\right\}$ and the optimum synthesis/design variables $\vec{x}_i^*$. It is possible to construct a surface of f^* versus the coupling functions u_{ij}. This hyper-surface constructed from the unit optimums is called the *Optimum Response Surface*[12] (ORS) of the overall synthesis/design problem.

The ORS is then used to define a system-level problem, which consists of finding the combination of coupling function values that lead to the minimum system level cost f^{**}. The system-level problem is in this case to:

minimize:

$$f^* = \sum_{t=1}^{\tau} \left(\dot{f}_1^* + \dot{f}_2^* + \dot{f}_3^*\right)\Delta t_t \qquad (13)$$

w.r.t. u_{ij_t} $\quad t = 1,...,\delta,...,\tau$

subject to:

$$\vec{H}_t = \begin{bmatrix} \xi_{ij} - \xi_{ij\,\max} \\ -\xi_{ij} + \xi_{ij_{\min}} \end{bmatrix}_t \le \vec{0};\ t = 1,..,\delta,..,\tau \qquad (13.1)$$

The local (unit-based) optimizations (e.g., problem (12)) can be performed in a nested fashion at the same time the system-level problem is being solved (Real Time LGO approach (RT-LGO)). A second alternative is to store the results from the sub-problems and use them later in the global (system-level) optimizer (Offline LGO approach (OL-LGO)). In both cases, the optimum results for the unit syntheses /designs form the ORS of the system.

It should be pointed out that the coupling function u_{ij} going from unit i to unit j may in fact be a vector of multiple products (e.g., electricity, steam, compressed air). It is clear then that a multi-unit, multi-product system may require a very large number of optimization runs (i.e. problems such as problem (12) would need to be solved innumerable times for many different combinations of the elements of the vectors u_{ij}). The potential problem caused by the large amount of computational and analysis time, which would be involved, is exacerbated by two facts:

- Each unit may need to be optimized using time decomposition (as described above).
- The synthesis/design problem in its entirety requires the use of binary, discrete and continuous variables. The optimization algorithms needed to deal with the resulting mixed-integer non-linear programming problems (MINLPs) are usually of the artificial intelligence type (e.g., Genetic Algorithm and Simulated Annealing). Although these algorithms are effective when properly developed and conditioned, they impose a serious computational burden on finding the solution.

Thus, the application of the LGO approach to complex, highly integrated, highly dynamic energy system synthesis/design may require a large number of optimizations to create the ORS. The amount of computational time required to do this may in some cases be impractical. A possible solution to these difficulties is the use of

[12] The optimum response surface (ORS) may be a graphical representation of the overall objective (constructed from the restricted unit-based minimum objectives) versus the coupling (intermediate feedback) functions, or it could also be a lookup table from which restricted optimum solutions can be obtained by interpolation, curve-fitting or other means. Furthermore, multiple optimum response surfaces exist any time an intermediate feedback is represented by a discrete instead of a continuous variable. However, in order to simplify our presentation, the singular tense will be used throughout even though more than one of these hyper-surfaces may be present for any given optimization problem.

the iterative version of the method (ILGO), which is presented below.

Although similar LGO based decomposition methods have been used in the past, those outside the field of thermoeconomics typically use components as the unit (as opposed to subsystems) along with first order objective functions. The objective functions commonly used are overall system efficiency at the system level and component adiabatic efficiency or mass at the unit level (e.g., Zimering et al., 1999). Although the use of LGO with these objectives is a vast improvement over typical trade-off analysis as practiced in industry, it is apparent that it does not fully account for all of the system-level effects that the component may have. In the case of a simple compressor, for example, the method will call for the maximization of the isentropic efficiency (for given inlet and outlet conditions) or minimization of mass (or cost). It is apparent, however, that the inherent competing tendencies of efficiency and mass (or cost) should be taken into account simultaneously and not separately. The LGO approach presented here does just that, taking into account both thermodynamic and size (economic) factors and their impact on the global (system) as well as local (unit) level objectives. An example application of the LGO method is described in detail in Muñoz and von Spakovsky (1999, 2000a).

2.4 Iterative local-global optimization (ILGO) approach applied to energy systems

The ILGO method uses the linear term of a Taylor series expansion to guide the selection of values for the coupling functions that make the system-level cost lower than that of some reference solution. Once a better solution is found the procedure is repeated until the optimum solution is achieved. ILGO starts by finding an arbitrary initial point on the ORS *without* actually creating the ORS[13]. This initial or reference solution is obtained by setting $u_{ij_t} = \xi^o_{ij_t}$ and solving a set of unit-level problems, which for unit 1 take the form:

minimize:

$$\dot{f}_1 = \sum_{t=1}^{\tau} \dot{f}_1\left(\vec{x}_1, \vec{y}_{1t}, \left(\xi^o_{21}, \xi^o_{31}, \xi^o_{12}, \xi^o_{13}\right)_t\right)\Delta t_t \quad (14)$$

w.r.t. $\vec{x}_1,\ \vec{y}_{1t} \quad t = 1,..., \delta,..., \tau$

subject to:

$$\vec{h}_{1t} = \vec{0} \quad t = 1,..., \delta,..., \tau \quad (14.1)$$

$$\vec{g}_{1t} \le \vec{0} \quad t = 1,..., \delta,..., \tau \quad (14.2)$$

As before, time decomposition may be needed to solve the above problem. The solutions to the unit-level sub-problems are the restricted local (unit-based) optimum cost rates at different times $\left(\dot{f}_i^*\right)^o_t$ and their corresponding restricted total values $\left(f_i^*\right)^o$ as well as the optimum operational decision variable values at various instants in time $\left(\vec{y}^*_{i\,t}\right)^o$ and the optimum design variable values $\left(\vec{x}_i^*\right)^o$ at the initial or reference point.

The initial value selection for the coupling functions ($u_{ij_t} = \xi^o_{ij_t}$) can be made in different ways. For example, an existing synthesis/design can be used as an initial point or a largely simplified model of the system can be used to find a near optimum solution, which could then be used as the ORS reference point. Another possibility is to use existing analysis techniques to find the coupling function values that cause the system, for example, to have a high Second Law efficiency.

Once a suitable initial or reference point on the ORS is found, a Taylor series expansion is performed about that point. After taking the linear term, the local (unit-based) cost rate at an instant of time t can then be written for unit 1 as:

$$\dot{f}_{1t} = (\dot{f}_1^*)^o_t + \left(\frac{\partial \dot{f}_1^*}{\partial u_{12}}\right)^o_t \Delta u_{12_t} + \left(\frac{\partial \dot{f}_1^*}{\partial u_{13}}\right)^o_t \Delta u_{13_t} + \left(\frac{\partial \dot{f}_1^*}{\partial u_{21}}\right)^o_t \Delta u_{21_t} + \left(\frac{\partial \dot{f}_1^*}{\partial u_{31}}\right)^o_t \Delta u_{31_t} \quad (15)$$

The partial derivatives above are by definition the shadow prices or marginal costs of the coupling functions. Similar quantities which have been defined in the past (e.g., von Spakovsky and Evans, 1993) form the basis of the calculus methods of thermoeconomics such as Thermoeconomic Functional Analysis (Frangopoulos, 1984, 1994), Engineering Functional Analysis (von Spakovsky and Evans, 1993; Evans and von Spakovsky, 1993; von Spakovsky, 1994) and the approach of El-Sayed (1989, 1996). The shadow prices (marginal costs) used here are more general in that they are defined for arbitrary coupling functions, energy or exergy based or not. Furthermore, the marginal costs in Eq. (15) are instantaneous and,

[13] It should be emphasized here that throughout the discussions on the ILGO approach (versions A and B), which follow, the ORS is never created. It is simply explored using marginal cost information (see discussions below).

thus, are allowed to take substantially different values at various instants in time.

Using the notation commonly found in the thermoeconomics literature, Eq. (15) is rewritten for units 1, 2 and 3 as:

$$\dot{f}_{1t} = (\dot{f}_1^*)_t^o + \lambda_{12t}^1 \Delta u_{12t} + \lambda_{13t}^1 \Delta u_{13} + \lambda_{21t}^1 \Delta u_{21t} + \lambda_{31t}^1 \Delta u_{31t} \quad (16)$$

$$\dot{f}_{2t} = (\dot{f}_2^*)_t^o + \lambda_{21t}^2 \Delta u_{21t} + \lambda_{23t}^2 \Delta u_{23t} + \lambda_{12t}^2 \Delta u_{12t} + \lambda_{32t}^2 \Delta u_{32t} \quad (17)$$

$$\dot{f}_{3t} = (\dot{f}_3^*)_t^o + \lambda_{31t}^3 \Delta u_{31t} + \lambda_{32t}^3 \Delta u_{32t} + \lambda_{13t}^3 \Delta u_{13t} + \lambda_{23t}^3 \Delta u_{23t} \quad (18)$$

where the marginal costs based on the restricted (unit-based) optimum local cost rate at an instant of time *t* are defined as:

$$\lambda_{ij}^i = \left(\frac{\partial \dot{f}_i^*}{\partial u_{ij}} \right)_t^o \quad (19)$$

and $$\lambda_{ji}^i = \left(\frac{\partial \dot{f}_i^*}{\partial u_{ji}} \right)_t^o \quad (20)$$

Quite naturally from the above definitions, "design" and "off-design" marginal costs can be defined. The former are those with $t = \delta$ and the latter those with $t \neq \delta$.

The equations presented above contain a wealth of information that can be exploited with the purpose of improving the initial or reference synthesis/design. They provide a means of moving in the optimum system cost vs. coupling functions (intermediate products/feedback) space, i.e. on the ORS. The first feature of these equations is that they show the trade-off between the costs that are purely local and those that are affected by synthesis/design and operational considerations in the rest of the system. The comparative magnitude of the λ's will indicate whether a decrease in intermediate coupling function values coming from unit i and the (likely) resulting increase in local cost of unit j will reduce the system-level cost. These marginal costs will, provided that they are not identically equal to zero[14], suggest synthesis/design changes that will make the system as a whole better from the standpoint of the cost objective. Thus, for example, negative marginal costs will point toward the need for higher values of the coupling functions (e.g., more of the intermediate products/feedbacks) and vice versa. Therefore, the optimizer would tend to favor syntheses/designs with greater values of the coupling functions but with lower associated marginal costs.

In addition, the off-design marginal costs become a measure of how important the entire load/environmental profile is when compared to the most critical point in the load/environmental profile, i.e. the synthesis/design point. The marginal costs will help pinpoint syntheses /designs that may have a relatively poor performance at the design point but may perform better than the best solution at the synthesis /design point when combined with all of the off-design conditions.

The step that follows the calculation of the marginal costs is problem dependent and leads to two different versions of the method: ILGO-A and B. Version A of the method (ILGO-A) uses the marginal costs as a guide for selecting a new set of values for the coupling functions. The descent algorithm for choosing these new values is given in detail in Muñoz and von Spakovsky (2000b,c) and is summarized as:

$$\left(\xi_{ij_t}^o \right)_{new} = \left(\xi_{ij_t}^o \right)_{old} - \alpha_o \left(\frac{\partial \dot{f}_{m\,t}^*}{\partial u_{ij}} \right)^o = \left(\xi_{ij_t}^o \right)_{old} - \alpha_o \lambda_{ij\,t}^m \quad (21)$$

where the marginal cost used in the above equation is such that the greatest improvement in the objective function is achieved. The step size, α_o, is chosen to ensure the descent properties of the algorithm.

The importance of Eq. (21) is that it shows the required changes in the coupling functions at all time steps so that both the synthesis/design and operational variables can be adjusted accordingly. It may be necessary, particularly for large problems, to perform the changes sequentially by using time decomposition. In ILGO-A a new set of values for the coupling functions at the synthesis/design point, i.e. $\left(\xi_{ij_\delta}^o \right)_{new}$, can be chosen according to Eq. (21). An improved solution at the synthesis/design point can be found by solving the decomposed (local or unit-based) optimization problems. The resulting set of most feasible solutions are then fed into the off-design problems to find the optimum operational variables. It is apparent that an implicit assumption in the use of ILGO-A is that there is enough confidence that an optimum solution can be obtained for the new values of the coupling functions $\left(\xi_{ij_t}^o \right)_{new}$ which may

[14] This would indicate that the reference point is in fact already the optimum for the objective consistent with the optimum for the system as a whole.

require some prior knowledge about system behavior[15]. After a new set of values for the coupling functions is chosen, the marginal costs are recalculated and the process repeated until nor further improvement is achieved or the physical limits of the independent variables are reached.

To circumvent the inherent drawback to ILGO-A noted above, a second version of the method, ILGO-B, has been developed. In this version, the coupling functions are allowed to fluctuate within limits to preserve the validity of the Taylor series expansion (as opposed to forcing them to take fixed values $\left(\xi^{o}_{ij_t}\right)$). ILGO-B improves upon the initial solution by solving a set of *unit-based system-level sub-problems*, which for unit 1 takes the form:

minimize:

$$f^{(1)} = \sum_{t=1}^{\tau} \begin{pmatrix} \dot{f}_1^* + \dot{f}_2^* + \dot{f}_3^* \\ +\lambda^1_{12_t}\Delta u^{(1)}_{12_t} + \lambda^1_{13_t}\Delta u^{(1)}_{13_t} \\ +\lambda^1_{21_t}\Delta u^{(1)}_{21_t} + \lambda^1_{31_t}\Delta u^{(1)}_{31_t} \\ +\lambda^2_{12_t}\Delta u^{(1)}_{12_t} + \lambda^3_{13_t}\Delta u^{(1)}_{12_t} \\ +\lambda^2_{21_t}\Delta u^{(1)}_{21_t} + \lambda^3_{31_t}\Delta u^{(1)}_{31_t} \end{pmatrix} \Delta t_t \qquad (22)$$

or

minimize:

$$f^{(1)} = \sum_{t=1}^{\tau} \begin{pmatrix} \dot{f}_1 + \dot{f}_2^* + \dot{f}_3^* \\ +\lambda^2_{12_t}\Delta u^{(1)}_{12_t} + \lambda^3_{13_t}\Delta u^{(1)}_{13_t} \\ +\lambda^2_{21_t}\Delta u^{(1)}_{21_t} + \lambda^3_{31_t}\Delta u^{(1)}_{31_t} \end{pmatrix} \Delta t_t \qquad (22.1)$$

w.r.t. $\vec{x}_1, \vec{y}_{1t} \quad t = 1,...,\delta,...,\tau$

subject to:

$$\vec{h}_{1_t} = \vec{0} \quad t = 1,...,\delta,...,\tau \qquad (22.2)$$

$$\vec{g}_{1_t} \le \vec{0} \quad t = 1,...,\delta,...,\tau \qquad (22.3)$$

Here, for example,

$$\Delta u^{(1)}_{12_t} = \nabla^T_{x_1} u_{12_t} \cdot \Delta\vec{x}_1 + \nabla^T_{y_1} u_{12_t} \cdot \Delta\vec{y}_{1_t} \qquad (23)$$

where the functional relationships given by Eq. (5) have been used. In general, the effect of the decision variables on the coupling functions is given by:

$$\Delta u^{(i)}_{ji_t} = \nabla^T_{x_i} u_{ji_t} \cdot \Delta\vec{x}_i + \nabla^T_{y_i} u_{ji_t} \cdot \Delta\vec{y}_{i_t} \qquad (24)$$

In addition to the above constraints, the additional constraints:

$$|\Delta u_{ij_t}| - \varepsilon\,|\Delta u_{ij_{t_{max}}}| \le 0 \qquad (25)$$

are imposed upon the problem. In expression (25), the $|\Delta u_{ij_{t\,max}}|$ are the maximum allowable values for the coupling functions and the factor ε is added to ensure that the linear Taylor series expansions are a good local representation of the ORS. It is readily seen that one of the advantages of ILGO-B over ILGO-A is that $\vec{x}_1$ and $\vec{y}_{1_t}$ may be chosen so that the internal (coupling) constraints (both for the analysis system of equations and for the desired unit's products or tasks) are *always* met. Another advantage is that unlike LGO, *neither* ILGO-A nor B requires nested optimizations.

Problem (22) represents the minimization of the system-level objective function by variations in the local (unit 1) decision variables only. The function to be minimized is composed of the local contribution (in this case f_1) to the overall objective *plus* the impact that the local decision variables ($\vec{x}_1, \vec{y}_{1_t}$) have on the local objectives of the other units (2 and 3). This impact is made via the coupling functions. Only one unit is used to carry out the optimization. This is made possible by the assumption that the marginal costs are correctly calculated. The solution of problem (22) will provide a new reference point on the ORS, which has a lower value of the system-level objective function than the previous reference solution. At this stage, the marginal costs are recalculated, and a new unit is chosen to perform optimization in the manner stated in problem (22). As with ILGO-A, the process is repeated until no further improvements are achieved or until the limits of the independent variables are reached.

The descent properties of the ILGO algorithm indicate that, at the very least, a local minimum will be found. This important finding leads us to conclude that if the cost function is convex and smooth with respect to the products and feedbacks, then the ILGO approach points toward a global optimum (e.g., the local minimum of a smooth convex function is the global minimum). In the worst case, the ILGO method only leads to a local minimum in which case the process must be repeated with different workable starting points (i.e. feasible syntheses/designs) until confidence in the solution as a global optimum is achieved. Despite the obvious time penalty that this may cause, the ILGO may still be the most if not the only practical optimization scheme that can be

[15] It should be noted that this cannot necessarily be guaranteed, hence ILGO-B.

applied to a highly complex, highly dynamic energy system synthesis / design.

The previous discussion allows one to tackle in an informed way the question of what thermodynamic property should be used as the coupling or communication variable between sub-problems (i.e. subsystems or components) when *physical decomposition* is used for optimization purposes. The authors believe that the answer depends on how the total cost function behaves with respect to the system's intermediate products and feedbacks (i.e. the ORS) when represented in terms of any of the candidate quantities (e.g., energy, exergy, thrust, negentropy, etc.)[16]. In fact, Gaggioli and El-Sayed, two of the biggest proponents of exergy and Second Law analysis, state in their landmark article of 1989 (Gaggioli and El-Sayed, 1989) that, for optimization, which quantity (ies) is (are) best is an open question and will more than likely depend on the case at hand. Of course, in the past, a number of authors have observed advantages to using exergy as opposed to energy, advantages, which they believed, simplified *decomposition* and speeded up and possibly even ensured convergence (Frangoupolos and Evans, 1984; Frangopoulos, 1984; Gaggioli and El-Sayed, 1989; von Spakovsky and Evans, 1993; Evans and von Spakovsky, 1993; El-Sayed, 1989, 1996). Furthermore, without *decomposition*, exergy has also been used as the basis for optimization algorithms, which guide the search for a global optimum by relating component or subsystem changes directly to improvements in the overall system objective (Tsatsaronis and Pisa, 1994). Clearly using exergy in the latter case is useful and clearly when the problem at hand is that of analysis and not optimization, exergy has any number of advantages in helping guide the synthesis/design in the most favorable direction (Sama, 1995). However, for optimization with *decomposition*, the need for exergy as the basis for the coupling or communication variable between sub-problems is only justified[17] on the basis of how, as stated above, the total cost function behaves with respect to the system's intermediate products/feedbacks and, thus, aids in *decomposition* and, in turn, optimization of the system as a whole. In certain cases, it will be the quantity of choice. In others, as has been shown (Muñoz and von Spakovsky, 1999, 2000 a, b, c; Frangopoulos, 1994; von Spakovsky, 1994), energy or some other quantity (e.g., thrust, negentropy, etc.) may work very well and be a better choice for any number of practical reasons.

Thus, based on the recent and past work of the authors and of others, the determining factor for which quantity (ies) is (are) the most appropriate is that of total cost function (overall system-level objective function) behavior with respect to the intermediate products and feedbacks, i.e.:

- that the ORS surface be smoothly convex (or concave) with respect to the products and feedbacks; this will ensure that the ILGO approach leads to the global optimum;
- that ideally the total cost function be linear with respect to these products and feedbacks; this will increase the convergence speed of the algorithm; obviously since the cost function is the sum of resources (usually fuel) and capital, there is always the alternative of manipulating the latter to make the cost function linear or piecewise linear, a technique which has been used by a number of researchers (e.g., Frangopoulos, 1984, von Spakovsky, 1986). A linear cost function with respect to the intermediate products and feedbacks would produce a hyper-plane and the optimum solution would be expected to be at or close to one of the corners of that plane.

Finally, some additional observations as to the best choice of thermodynamic quantities for describing the intermediate products and feedbacks of a system can be made:

- Consider a single unit that uses a single resource R_1 to produce a single product P_1. The synthesis/design optimization will find the optimum vector of decision variables $\vec{X}_1^{**}$ and $\vec{Y}_1^{**}$ that minimize the sum $k_1R_1 + Z_1$ for a given value of P_1. Typically, if the quantity or quality of product P_1 increases, the best design will tend to have a higher value for the total cost function than that of a synthesis/design with a lower required P_1. This is valid regardless of the choice of thermodynamic property used to describe the product. The implication is that overall (total) cost functions have the tendency to be *monotonic* with respect to their products. This type of behavior will favor the convexity of the cost function. Problems arise, however, when the need to have a larger product forces changes in the technology being employed. In this case the tendency may be inverted and even make the

[16] This has direct bearing on the associated marginal costs and their behavior.

[17] Of course, using exergy may add information which otherwise would not be there and could eventually aid in an interpretation of the optimization results. The argument made here, however, is that exergy is simply not necessarily required in order to obtain these results using *decomposition*.

total cost function discontinuous. This obviously can occur when the overall optimization problem uses a discrete variable that represents various possible types of units (a vapor compression cycle vs. an absorption cycle, for example). Note, however, that discrete variables present in the local (unit) optimization problem (e.g., representing different types of material for a given component) do not pose this problem.

- Exergy has the important mathematical characteristic of combining temperature, pressure, chemical composition, velocity, mass flow rate, etc. in a single function. This conceptually poses an advantage for the calculation of the shadow prices (marginal costs). A fair amount of work has been devoted to the study of exergy-based marginal costs in stationary applications (Serra, 1994; Frangopoulos, 1994; von Spakovsky, 1994; Lazzaretto and Andreatto, 1995; etc.). However, there are practical difficulties for their calculation when models of real systems are used. For example, take the case of the design of a gas turbine, which in addition to shaft work produces compressed air for a process. The air is to be taken, say, from the last compressor stage. It is much easier to design the system for a given value of the air mass flow rate to be taken from the compressor than for a given exergy value. This is because the pressure and temperature of the air depend on a number of factors that are not easily controllable, including, among others, the position of the design point on the gas turbine maps, the maximum allowable temperature in the combustor, the technology used and some stability considerations.
- There is a need to remain open-minded to the possibility of using marginal costs based on commodities other than exergy or energy*[17]. In some applications, the use of non-energy values may be necessary. For example, size (volume and mass) and thrust (force) are critical factors in aircraft design. Although some authors (Frangopoulos and von Spakovsky, 1993; von Spakovsky and Frangopoulos, 1994; Sciubba, 1999) may argue that one could relate exergy to a unit's mass via, for example, the manufacturing process, that option is replete with difficulties and pitfalls (Curti et al., 2000 a, b) and will simply not be considered here.

3. Conclusions

The methods presented in this paper constitute a natural way for carrying out the decomposed synthesis/design optimization of highly coupled, highly complex energy systems. The Local-Global Optimization (LGO) approach in any of its forms (Real-time or Off-line) with its associated Optimum Response Surface (ORS) constitutes a powerful way of not only obtaining a global optimum solution but of gaining an enormous amount of insight as to the relative effect that each unit has in terms of the overall objective. The potentially large investment required for LGO is addressed by the iterative version of the approach, ILGO, which requires no nested optimizations and uses an approximation of the ORS to reduce the number of unit optimizations required. The effect of the different units' independent variables is assessed in terms of the local (unit-based) cost *and* their effect on the rest of the system. Thus, in ILGO-B, unit-based system-level optimization sub-problems (as opposed to purely local objective functions) are defined. Each of these sub-problems, while using strictly local (unit) independent variables, approximates the system-level optimum cost. The approximation of the ORS leads to the definition of shadow prices (marginal costs) as the partial derivatives of the optimum cost with respect to the functions connecting the units. One of the most appealing features of ILGO is its ability to provide the information necessary to improve an existing design. In fact, in engineering practice, the word optimization is often used not to indicate the search for an absolute global optimum but rather to find a solution, which is *better* than some existing system. Any of the versions of ILGO excels at this task since one could use the existing design (which is assumed to be "optimized") as the reference condition and start the iterative process from there.

The approaches presented in this paper, while mathematically rigorous, have two great practical advantages. First, they permit the mathematical handling and solution of very large optimization problems by defining mutually consistent smaller sub-problems. Second, the fact that *decomposition* is done across unit boundaries allows the method to fit perfectly with current multi-/inter-disciplinary engineering design practices.

In addition to the above, the approaches presented shed some light on the on-going controversy as to the importance and usefulness of Second-Law based methods *for the synthesis/ design optimization* (as opposed to analysis) of

[17] Other functions have been proposed and used in the past. For example, Valero et al. (1993) proposed the use of the relative free energy.

energy systems. There is no doubt that Second Law methods as *analysis* tools are superior to First Law approaches. However, when it comes to *optimization*, this is not necessarily true. Once the optimization problem is defined, there is only one global optimum and whether or not the problem is represented in Second or First Law terms has no effect on this optimum. Thus, the question becomes: is a Second Law *decomposition* approach superior to a First Law approach in arriving at the optimum? Again, the answer is: not necessarily. In our view, whether or not one defines the problem in terms of the Second or First Law should depend on what effect the "properties of choice" for representing intermediate products and feedbacks has on the mathematical behavior of the ORS. Thus, properties that lead to monotonic and, in the ideal case, linear behavior of the optimum cost in the intermediate products/feedbacks domain are preferred, whether they are exergy-based or not. As will be seen in the accompanying paper (Muñoz and von Spakovsky, 2001) in which the ILGO approach is applied to a large-scale optimization problem, the desirable "properties of choice" were not Second Law based.

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Nomenclature

d	Number of design variables
$\dot{f}$	Rate form of the objective function
f	objective function
$\vec{G}, \vec{g}$	vector of inequality constraints
$\vec{H}, \vec{h}$	vector of equality constraints
k	constant, conversion factor
o	number of operational variables
P, p	product
R, $\dot{R}$	external input (resource), rate form
$\vec{X}, \vec{x}_i$	vector of design variables
$\vec{Y}, \vec{y}_{i_t}$	vector of operational variables
u_{ij}	coupling (intermediate feedback) function
Z	capital function (e.g., cost, weight, volume)

Greek symbols

α	step size
δ	design point
ε	small number
λ	shadow price (marginal cost)
τ	number of time segments into which the set of load/environ-mental conditions is divided
ξ	coupling (intermediate feedback) function value

Superscripts

fp	feasible and "promising" solution
o	reference, initial value
p	capital
*	restricted optimum
**	Unrestricted (global) optimum

Subscripts

o	reference, initial

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