INTEGRATION OF A THERMODYNAMIC PROCESS SIMULATOR WITH GENETIC OPERATORS FOR MATHEMATICAL EXERGOECONOMIC OPTIMIZATION OF THERMAL SYSTEMS

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Abstract. *In this article we present the implementation of an integrated approach to perform mathematical exergoeconomic optimization of thermal systems based on genetic operators. While genetic algorithms will less likely stop at local optima than gradient search methods, they tend to be computationally expensive. For these reasons, in our approach, genetic operators are integrated with a thermodynamic process simulator. With this strategy, the computational power of the simulator is fully exploited, such that the optimization procedure may disregard the variables associated with the thermodynamic balance equations, and thus deal with the decision variables only. We demonstrate the potential of this integrated approach through application to a model cogeneration system. The conventional optimization of the system would require the manipulation of* $O(10^2)$ *variables, whereas the integrated procedure has to deal with only 5 decision variables in the optimization kernel. Because the thermodynamic balance equations are decoupled from the optimization routine, the proposed approach is computationally efficient, and it can be employed to optimize thermal systems as complex as the simulator will allow.*

Keywords: *process simulator, genetic operators, exergoeconomics, optimization, thermal systems*

1. Introduction

A crucial economical issue for modern societies is the efficient utilization of natural energy resources, which explains the recent increase in the development of techniques for energy systems optimization worldwide. Besides the push for efficiency, there is also a strong demand for reducing harms to the environment, and for achieving sustainable development (Rosen and Dincer, 2001). In this context, the techniques of exergoeconomics can address environmental issues, reveal the cost formation process of system products, and aid system optimization. Reviews of the field of exergy and exergoeconomic analysis can be found in the works by Tsatsaronis (1993), Donatelli (2002), Vieira (2003), and Frangopoulos (2003). In Brazil, research in the exergoeconomic arena has focused mostly on the evaluation and interpretation of different cost partition methodologies (e.g., Júnior and Hombeeck, 1997; Vieira and Júnior, 1998; Cerqueira and Nebra, 1999; Antunes and Silveira, 1999; Balestieri *et al*., 1999; Donatelli *et al*., 2000; Gallo and Gomes, 2003; Júnior and Arriola, 2003), as opposed to the development and application of exergoeconomic *optimization* techniques to thermal systems. To evaluate and compare different exergoeconomic methodologies, *C*. Frangopoulos, *G*. Tsatsaronis, *A*. Valero, and *M*. von Spakovsky have proposed the optimization of the *CGAM* five-component cogeneration system (Tsatsaronis, 1994) as a benchmark problem, which gained wide acceptance thereafter.

It is a fact that exergoeconomics provides insights to system optimization (Bejan *et al*., 1996). However, to actually perform exact system optimization, the application of a mathematical optimization technique is required. In general, when a conventional mathematical optimization technique is applied to a thermal system, the thermodynamic balance equations and the component model equations are formulated as restrictions in the optimization problem. Furthermore, these equations must be explicit, and the involved variables must be treated together with the decision variables, thus significantly increasing the dimension of the problem. Considering that the thermodynamic simulation of real systems requires a large number of variables, the conventional mathematical optimization of a thermal system is, indeed, a large-scale problem (Jaluria, 1997). Actually, even for simulating the relatively simple CGAM cogeneration system, $O(10^2)$ variables are required (the number of variables rapidly increases as better thermodynamic models are used).

To circumvent the difficulties associated with the application of conventional mathematical optimization techniques to real thermal systems, exergoeconomic approaches have recently been developed, which require the determination of the costs within the system. As discussed in Vieira *et al*. (2004), system costs can be determined through either algebraic or calculus methods. Many exergoeconomic optimization techniques employ calculus methods, due to these methods intrinsic characteristics, usually based on Lagrange multipliers (Jaluria, 1997). Still, because the optimization of complex systems is a non-trivial task, it is crucial to integrate optimization algorithms with a professional thermodynamic process simulator. In this manner, not having to deal with the mass, energy, and exergy (or, entropy) balance equations, the optimization task gains significant efficiency. Motivated by the facts that it is not always possible to obtain explicitly the thermodynamic balance equations, and that in practice the system to be optimized is already modeled in a process simulator, in this paper we present the implementation of an integrated approach for thermal systems optimization, and apply it to the benchmark CGAM cogeneration system. The approach has been conceived, in fact, to optimize real complex thermal systems: it fully exploits the computational power of a professional process simulator, and it deals, in the optimization kernel, with a reduced set of variables, while the thermodynamic requirements are completely realized by the simulator. This computationally advantageous strategy, however, might lead to eventual errors in the simulator, due to choices for the values of decision variables in the optimization routine which would force violation of the laws of thermodynamics. To avoid program crashes in these instances, the objective function is penalized in the optimization routine.

While any mathematical optimization method can be implemented in the integrated approach, a 'derivative-free' method should be favored, because in general evaluations of derivatives cannot be guaranteed. In this work, the chosen method is the robust genetic algorithm, developed originally by Holland (1975). The selected professional process simulator is the IPSE-pro system, version 3 (SimTech, 2000). For costing purposes, the methodology SPECO/AVCO (Lazzaretto and Tsatsaronis, 1999) is adopted. The integrated approach is relatively easy to implement, and it can be employed to optimize thermal systems as complex as the simulator will allow. The results which we obtain for the CGAM system are presented and analyzed, and show the potential of our approach.

2. Integration with the Process Simulator

The present integrated exergoeconomic optimization technique exploits the power of the IPSE-pro process simulator, details of which can be found in Vieira (2003) and Vieira *et al.* (2004). In this work, IPSE-pro includes the simulator module PSE coupled to the modules MDK (Model Development Kit), PSE-Excel, and the Advanced Power Plant Library (APP-Lib). APP-Lib contains models of thermal systems components, and with MDK one can incorporate the exergy property calculation into the simulator. Through the DDE (Dynamic Data Exchange) protocol, the PSE-Excel module permits integration of the optimization routine with the simulator; the routine must be coded with the programming language Visual Basic for Applications (VBA). Also, through Excel worksheets, it is possible to exchange variables between the VBA routine and IPSE-pro. Control of data exchange is performed using Excel macros.

The simulator determines all mass, energy, and exergy flow rates of the system, and it is called by the optimization routine each time a modification of any decision variable is necessary. To prevent failure of the integrated algorithm due to errors caused by selection of unfeasible thermodynamic data in the VBA routine, a penalty value is added to the value of the objective function, whenever IPSE-pro sends an error code back to the VBA routine. Note that the optimization routine does not have to deal with the thermodynamic balance equations as restrictions.

The integrated approach allocates great part of the computational effort to the simulator. Total computational time is thus (roughly) proportional to the number of evaluations by the simulator. A direct optimization method – a genetic algorithm (Holland, 1975) – has been selected (Mothci, 2005), as opposed to (not-so-straightforward) gradient methods. In addition, the robustness of a genetic algorithm suggests that it might be a good alternative to the flexible polyhedron method used by Vieira (2003) and Vieira *et al.* (2004). In the latter works, the authors report that the flexible polyhedron method (Himmelblau, 1972) has the inconvenience of requiring several restarts (with different initial polyhedra) in the course of an optimization process.

3. The Genetic Algorithm

Genetic algorithms (Holland, 1975) are mathematical optimization methods based on the biological principle of natural selection, which warrants survival of the fittest individuals of a given population. Usually, the aptitude of an individual is represented quantitatively by the associated value of the objective function, such that at the end of the optimization process the fittest individual constitutes the problem optimal solution. From an initial random population, natural selection works its way thru generations, modifying the individuals by means of crossover and/or mutation, leading to new populations. The steps of a genetic algorithm are illustrated in Figure 1.

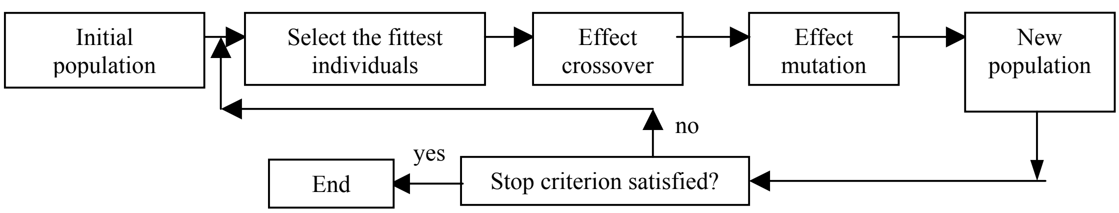

Figure 1. Steps of a genetic algorithm.

Traditionally in genetic algorithms, an individual is represented by a chain of bits (0's and 1's), which forms the chromosome containing all the information necessary to measure the fitness of the individual. Due to the widths of the allowable ranges for the decision variables in the CGAM problem, here we have coded the chromosomes with real numbers (i.e., adopted the so-called real coding), as illustrated in Figure 2. To decrease the number of calls to the simulator, and thus to save computational time, each chromosome is made to possess information about the decision variables (*DV*1 to *DV*5) and the objective function (*OF*). Accordingly, the classical genetic operators of crossover and mutation have had to be modified, i.e., implemented with real coding too. To improve the performance of the algorithm, and to avoid stochastic errors due to pseudo-random number generation, the elitism operator has also been used, which guarantees that the fittest individual in a given generation will be present in the following generation.

OF	*DV*1	*DV*2	*DV*3	*DV*4	*DV*5

Figure 2. Real coding of the chromosome of an individual.

The performance of genetic algorithms with respect to convergence to the global optimum point in the search space depends on the values assigned to the various control (adjustable) parameters. The size of the population (i.e., its number of individuals), N_p, and the probability of occurrence of a mutation, P_m, are two such parameters associated with the diversity of the population. The greater the diversity, the greater are the chances that some individual will be close to the global optimum of the objective function. The population diversity is maximum at the beginning of the genetic-algorithm search process, and decreases along the generations. The probability of occurrence of a crossover, P_c, and the method of selection, on the other hand, determine the selection pressure of the genetic algorithm. The selection pressure is responsible for guiding the search to promising regions of the space. The larger the selection pressure, the larger is the speed of convergence to such regions. Because of the somewhat competing tendencies just described, a parametric study has been carried out (Mothci, 2005), to judiciously adjust the values of all the control parameters to be used in the optimization processes to be performed with the genetic algorithm. Table 1 presents the chosen values.

Table 1 – Values of the control parameters of the genetic algorithm to optimize the CGAM system.

Parameter	**Variable**	**Value**
Population size	N_p	200
Maximum number of generations	G_{max}	80
Probability of occurrence of a crossover	P_c	65%
Probability of occurrence of a mutation	P_m	5%

4. Application to the CGAM System

Application of the present integrated optimization approach to the benchmark CGAM cogeneration system (Tsatsaronis, 1994) is described in the next four subsections.

4.1. The CGAM System

The CGAM system, shown in Fig. 3, is a cogeneration system that produces fixed amounts of electrical power and saturated steam. The electricity production is 30 MW, and the saturated steam mass flow rate at 20 bar is 14 kg/s. The CGAM system consists of the following 5 components: air compressor, air preheater, combustor, gas turbine, and heat recovery steam generator (HRSG). The combustor fuel is natural gas with a lower heating value of 50000 kJ/kg.

It is important to remark that the physical, thermodynamic and economic models used in this paper are different from those of the original CGAM problem (Tsatsaronis, 1994). Here, the physical and thermodynamic models are solved with the IPSE-pro program, not through simplified balance and property equations. The exergy-based economic model consists of component cost equations derived from fits to data points obtained from the original CGAM cost equations (Vieira, 2003). Because of these differences, the results presented in section 5 cannot be directly compared to the results shown in the original reference (Tsatsaronis, 1994). In the next subsection, the cost equations used in this work are reported.

4.2. Cost Equations

The main costs of a thermal system are the capital investment cost, the operation and maintenance cost, and the fuel cost. In the literature, a simplification of the Revenue Requirement Method (Bejan *et al*., 1996) is often used to perform the economic analysis. A simplified economic model is thus assumed, which is based on the capital recovery factor (*CRF*), and considers that the total capital investment (*TCI*) in a plant is given by the sum of all the purchased-equipment costs (*PEC*) multiplied by a factor β (Bejan *et al*., 1996), as expressed by

$$TCI = \sum_k TCI_k = \sum_k \beta\, PEC_k = \beta \sum_k PEC_k = \beta\, PEC\,, \tag{1}$$

where $k = 1,\ldots,NK$ is the index for the component (or individual equipment), and NK is the total number of components in the plant. The capital recovery factor (*CRF)* is expressed by

$$CRF = \frac{i(1+i)^{\ell}}{(1+i)^{\ell} - 1}\,, \tag{2}$$

where ℓ and i are, respectively, the useful system life and interest rate.

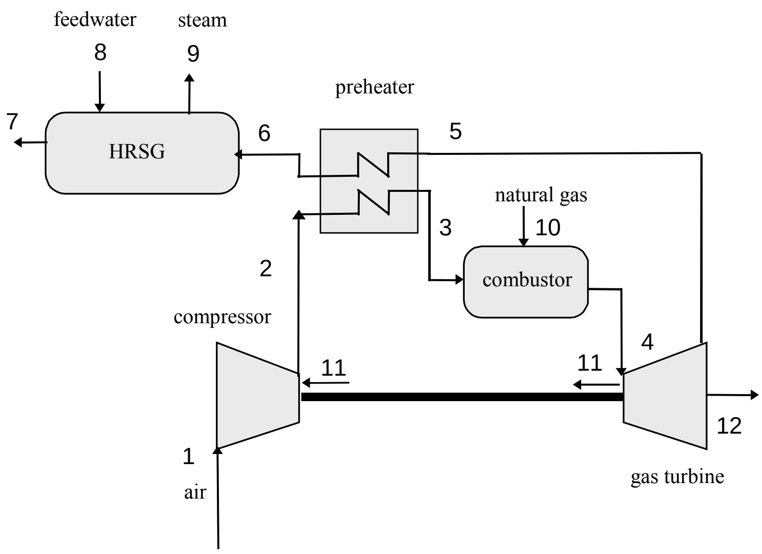

Figure 3. The CGAM cogeneration system (HRSG is the heat recovery steam generator).

The system total cost rate excluding fuel costs, $\dot{Z}$, is the sum of the investment and the operation and maintenance costs for all components, and is expressed by

$$\dot{Z} = \sum_{k=1}^{NK} \dot{Z}_k = \frac{\left(\sum_{k=1}^{NK} CRF(1+\gamma)\, TCI_k \right)}{\tau}\,, \tag{3}$$

where τ is the yearly plant operating hours, and γ is the maintenance factor, here assumed constant. The fuel cost flow rate $\dot{C}_F$ is expressed by

$$\dot{C}_F = c_F \dot{m}_F LHV\,, \tag{4}$$

where c_F, $\dot{m}_F$, and *LHV* are the fuel (i.e., natural gas) specific exergetic cost, mass flow rate, and lower heating value, respectively.

The purchased-equipment cost for component k, PEC_k, is expressed by

$$PEC_k = B_k \left(\frac{\varepsilon_k}{1-\varepsilon_k} \right)^{n_k} \dot{E}_{P,k}^{m_k} . \tag{5}$$

In Eq. (5), ε_k and $\dot{E}_{P,k}$ are the exergetic efficiency and product exergy flow rate of component k, respectively, and B_k, n_k and m_k are fitting parameters. For the gas turbine and combustion chamber of the CGAM system, however, to correctly evaluate the strong effect of the combustion chamber outlet temperature T_4 on the component costs, Eq. (5) must be slightly modified to read

$$PEC_k = B_k \exp\left(B_{k1} T_4 + B_{k2}\right) \left(\frac{\varepsilon_k}{1-\varepsilon_k} \right)^{n_k} \dot{E}_{P,k}^{m_k} . \tag{6}$$

In order to obtain all the expressions for the purchased-equipment costs, each component k is simulated individually with the IPSE-pro program, such that the exergetic efficiency and product exergy flow rate are calculated for many different input operating conditions. With this procedure, aided by efficient nonlinear estimation techniques available with the Statistica 5.0 program (StatSoft, 1996), Vieira (2003) obtained the values, shown in Table 2, of the parameters B_k, B_{k1}, B_{k2}, n_k and m_k in Eqs. (5) and (6) for the CGAM system components.

Finally, the values of the economic parameters used in all the present calculations are (Vieira, 2003; Bejan *et al.*, 1996): $\beta = 6{,}32$, $\ell = 10$ years, $i = 12.7\%$, $\tau = 8000$ hours, and $\gamma = 0.06$.

Table 2 – Values of parameters for purchased-equipment cost equations, Eqs. (5)-(6).

Component	B_k	B_{k1}	B_{k2}	n_k	m_k
compressor	51.9	-	-	2.499	1.002
combustor	299.9	0.014	-19.898	1.038	1.002
gas turbine	181.3	0.035	-53.799	1.450	1.004
HRSG	98645.7	-	-	0.783	0.649
preheater	44839.1	-	-	0.917	0.371

4.3. Exergoeconomic Analysis

An exergoeconomic analysis of the CGAM cogeneration system is performed. Therefore, as detailed in Tsatsaronis (1993, 1994), Bejan *et al.* (1996), and Vieira (2003), for each component k, $k = 1,\ldots,NK$, the following quantities must be calculated: exergy destruction flow rate ($\dot{E}_{D,k}$), component exergetic efficiency (ε_k), exergy destruction and exergetic cost flow rates (respectively, $\dot{C}_{D,k}$ and $\dot{C}_k$), component product and fuel specific exergetic costs (respectively, $c_{P,k}$ and $c_{F,k}$), and component investment cost flow rate ($\dot{Z}_k$). The fuel and product of each component are calculated as proposed by Lazzaretto and Tsatsaronis (1999). Also, component cost partitioning obeys the rules for fuel and product stated in Lazzaretto and Tsatsaronis (1999). To actually perform the cost calculations, the incidence, fuel, product, and cost matrices are determined following the Theory of the Exergetic Cost (Lozano and Valero, 1993). For the CGAM system, the input specific exergetic cost flow rates are known. The fuel cost is 14.40 US$/MWh. The air for combustion and the water for the HRSG are not charged.

4.4. The Optimization Problem

The objective function to be minimized in the optimization problem is the sum of the specific costs of the products (i.e., summation of the plant investment, operation and maintenance costs and the fuel costs). For the CGAM system, specifically, because there is only one fuel and the products are constant, the objective function OF can be given equivalently by

$$OF = \dot{C}_{total} = \sum_{k=1}^{NK} \dot{Z}_k + \dot{C}_F = \frac{\left(\sum_{k=1}^{NK} CRF(1+\gamma) TCI_k \right)}{\tau} + c_F \dot{m}_F LHV \; . \tag{7}$$

As previously mentioned, the process simulator determines all the mass, energy, and exergy flow rates throughout the system. As opposed to a conventional mathematical optimization procedure, the integrated approach does not require that the thermodynamic balance equations and the component model equations be written explicitly as restrictions of the problem. For the CGAM-system optimization problem as described in this section, Table 3 shows the chosen decision variables and their limiting values.

Table 3 – Decision variables and their limiting values.

Variable description	**Variable symbol**	**Lower / upper limit**
compressor pressure ratio	*RPc*	7 / 27
combustor inlet temperature	T_3 (°C)	427 / 827
combustor oulet temperature	T_4 (°C)	827 / 1227
compressor isentropic efficiency	η_{AC}	0.7 / 0.9
gas turbine isentropic efficiency	η_{GT}	0.7 / 0.9

5. Results and Discussion

In this section, the results obtained with the application of the mathematical optimization routine integrated with the IPSE-pro process simulator to the CGAM system is presented and analyzed.

Table 4 displays the final values of the decision variables and the final values of the objective function for both the genetic algorithm (GA, 2nd column) and the flexible polyhedron method (FPM, 3rd column). The values obtained with the flexible polyhedron method are taken from the monograph by Vieira (2003). Table 4 also displays the relative differences δ (4th column) and μ_i (5th column), respectively given by

$$\delta = \frac{\left| OF - OF_{fpm} \right|}{OF_{fpm}} \times 100\% \, , \tag{8}$$

and

$$\mu_i = \frac{\left| X_{i,f} - X_{i,fpm} \right|}{X_{i,fpm}} \times 100\% \, , \quad i=1,...,n. \tag{9}$$

In Eq. (8), OF_{fpm} is the final value of the objective function for the flexible polyhedron method. In Eq. (9), $X_{i,f}$ is the final value of decision variable X_i, and $X_{i,fpm}$ is the final value of decision variable X_i for the flexible polyhedron method.

Table 4 – Final values of the decision variables and objective function for the genetic algorithm (GA) and the flexible polyhedron method (FPM).

Variable name	GA	FPM	δ(%)	μ_i (%)
RPc	8.198	8.201	–	0.04
T_3 (°C)	589.9	609.0	–	3.14
T_4 (°C)	1218.8	1227.0	–	0.67
η_{AC}	0.880	0.873	–	0.80
η_{GT}	0.843	0.838	–	0.60
$OF = \dot{C}_{total}$ (US$/h)	1652.71	1647.01	0.35	–

We observe from the data in Table 4 that the largest values of δ and μ_i are 0.35% and 3.14%, respectively. For engineering purposes, in view of these small discrepancies found for the final values of the objective function and decision variables, we can assert that the genetic algorithm effectively reached the minimum for the CGAM problem.

The integration of the genetic algorithm (Holland, 1975) with the IPSE-pro process simulator (SimTech, 2000) permits the optimization routine to handle just the decision variables, saving time in the optimization kernel (as compared to a conventional approach without employing the simulator). Because the number of variables dealt with by the optimization routine is relatively small (5) with respect to the number of variables required for system simulation ($O(10^2)$), the total CPU time for executing the optimization process depends mainly on the time demanded by the simulator, which scales with the number of simulation variables. Here, the end result is that the computational time of the methodology is (roughly) proportional to the number of calls to the simulator.

The computational time of the genetic algorithm is greater than that of the flexible polyhedron method. This fact is due to the characteristic that the genetic algorithm works along the optimization process with many points, the so-called potential solutions. Effectively, the unfolding of the problem solution – the global optimum point – occurs at the last generation with the choice of the best individual. At the end of an optimization process, using the values specified in Table 1 for the control parameters, the number of calls to the simulator by the genetic algorithm is 16000, equal to the product of the population size by the maximum number of generations. As a consequence, for the CGAM cogeneration system, the average CPU time for complete optimization is 7 hours on a Pentium III 750 MHz/256 Mb RAM computer. On the other hand, as reported by Vieira (2003), the flexible polyhedron method calls the simulator 2414 times, with a corresponding computational time of about 1 hour. Nevertheless, the genetic algorithm does not require successive restarts of the optimization process, as does the flexible polyhedron method (Vieira, 2003). This is a significant advantage if one wishes to apply the integrated exergoeconomic approach to complex thermal systems (see below).

6. Closing Remarks

Thermodynamic simulation programs are widely used for designing real thermal systems, but most of them do not incorporate second law optimization techniques. In this study, an integrated approach has been implemented, which integrates a well-known mathematical optimization method with a professional process simulator, so as to be able to perform exergoeconomic optimization of complex thermal systems. The selected mathematical method is the genetic algorithm, and the process simulator is the IPSE-pro system. All costs are calculated on an exergy basis. As a demonstration exercise, the proposed approach is here applied to the CGAM benchmark cogeneration system.

A conventional mathematical optimization approach applied to the cogeneration system treated in this work, but not using a simulator and adopting simplified mass, energy and entropy balances as restrictions in the optimization problem, would require the manipulation of $O(10^2)$ variables. Integration of the mathematical method with the simulator permits a reduction in the number of variables dealt with by the optimization routine by two orders of magnitude.

The integrated approach has proved effective: the coupling of the mathematical algorithm to the simulator does lead to the optimization of the CGAM thermal system. The discrepancy in the final values of the objective function for the genetic algorithm and for the flexible polyhedron method is below the small margin of 0.35%, fully acceptable in engineering practice. These results highlight the potential of the present integrated approach to handle real complex thermal systems. In fact, it is expected that the performance of the genetic algorithm – CPU time – will improve relative to that of the flexible polyhedron method as more complex problems are tackled. The reason is that the number of simulator calls will increase significantly for the latter method, but very little for the former.

Finally, we suggest that, to improve the performance of the genetic algorithm, hybrid methods be used, such as the Meta-AG (Grefenstette, 1986). The Meta-AG uses, along the optimization process, another independent genetic algorithm to adjust the values of the parameters for the probabilities of crossover, P_c, and mutation, P_m. The advantage of such procedure is that smaller population sizes can be used, because the diversification of the potential solutions (individuals) is warranted by the optimal parameters (mainly P_m), not population size.

7. Acknowledgements

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