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Multiobjective Optimization of Utility Plants under Several **Environmental Indicators Using an MILP-Based Dimensionality Reduction Approach**

P. Vaskan, †,‡ G. Guillén-Gosálbez, *,†,§ M. Turkay, and L. Jiménez

ABSTRACT: We address the multicriterion optimization of utility plants with economic and environmental concerns. Rather than optimizing a single environmental metric, which was the traditional approach followed in the past, we focus on optimizing these systems considering simultaneously several environmental indicators based on life cycle assessment (LCA) principles. We combine a multiobjective optimization model with an MILP-based dimensionality reduction method that allows identifying key environmental metrics that exhibit the property that their optimization will very likely improve the system simultaneously in all of the remaining damage categories. This analysis reduces the complexity of the underlying multiobjective optimization problem from the viewpoints of generation and interpretation of the solutions. The capabilities of the proposed method are illustrated through a case study based on a real industrial scenario, in which we show that a small number of environmental indicators suffice to optimize the environmental performance of the plant.

1. INTRODUCTION

The adoption of more sustainable technologies in industry is a central topic in sustainability and green engineering. Particularly, the design and planning of efficient energy systems capable of satisfying a given power and steam demand has recently gained wider interest in this field.1

Several methods are available in the literature for the synthesis of utility plants. They can be classified into two main groups. The first are based on thermodynamic targets and heuristics.^{2,3} As pointed out by Bruno et al.,⁴ their main drawback is that, even if the design with highest thermal efficiency is obtained, it may not be economically attractive because capital costs may be too high. The second group, to which the present work belongs, relies on rigorous optimization techniques based on mathematical programming (i.e., linear programming (LP), nonlinear programming (NLP), mixedinteger linear programming (MILP), and mixed-integer nonlinear programming (MINLP)). Optimization approaches based on LP and MILP techniques were originally introduced in this area by Nishio and Johnson⁵ and Papoulias and Grossman.⁶ Later on, Hui and Natori⁷ developed an MINLP model for the optimal operation of site utility systems, while Bruno et al.⁴ proposed an MINLP formulation for the design of utility systems. Soylu et al.8 and Luo et al.9 developed MILP models for the integration of different utility systems for the minimization of the cost and environmental impact.

These strategies have traditionally focused on optimizing the utility plant considering the economic performance as unique criterion and disregarding the environmental impact. 4,10 An alternative approach to the single-objective optimization

consists of posing the design task as a multiobjective decision-making problem that explicitly considers environmental concerns. This approach allows identifying solutions in which the economic and environmental performances are simultaneously optimized.

A key point in the use of multiobjective optimization as applied to the development of more sustainable processes concerns the assessment of the environmental performance of the system. Among the tools available, life cycle assessment (LCA) has recently gained wider attention in the environmental engineering community. The integration of LCA and multiobjective optimization results in a powerful quantitative tool that facilitates the environmentally conscious design and planning of industrial processes.

Stefanis et al. 11,12 were the first to propose the combined use of multiobjective optimization (MOO) and LCA principles. In the recent past, this approach has been applied to a wide variety of industrial problems, such as the design of chemical plants, 13,14 the strategic planning of supply chains, 15-17 the analysis of biodiesel production, ¹⁸ the design of heat exchanger networks ¹⁹ and solar energy plants, ²⁰ the eco-design of buildings, ²¹ and the design and planning of energy systems, ¹

Defining a suitable LCA metric to drive the optimization of an energy system is of paramount importance. A plethora of

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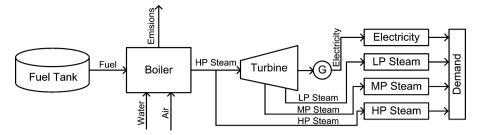


Figure 1. Energy system taken as reference.

LCA-based indicators are nowadays available for quantifying the impact in several damage categories. The simultaneous optimization of all of them would lead to highly complex models that would be very hard to solve. This is because the generation and analysis of the Pareto points of a model becomes more difficult as we increase the number of objectives. A deeper discussion of this point can be found in the work by Copado et al.²²

The prevalent approach for overcoming this limitation is to use aggregated metrics that translate several environmental metrics into a single indicator defined by assigning weights to them. Following this approach, most authors have developed bicriteria models where the economic performance is traded off against a single environmental indicator obtained as a weighted sum of individual impacts. ^{23,24} This approach simplifies the analysis to a large extent, but has two main drawbacks. The first is that the weights used may not necessarily reflect the preferences of decision-makers. The second is that their optimization might change the structure of the problem, in a manner such that some optimal solutions might be left out of the analysis. ²⁵

Multidimensionality reduction methods aim to overcome these limitations.²⁶ They allow identifying redundant objectives that can be omitted while still preserving the problem structure to the extent possible. Particularly, Deb and Saxena²⁷ were the first to investigate dimensionality reduction in MOO. They developed a statistical method based on principal component analysis (PCA) for eliminating nonessential objectives in MOO problems, thereby simplifying the associated calculations. Brockhoff and Zitzler (2006)²⁸ proposed an alternative dimensionality reduction approach based on identifying those objectives whose elimination simplifies significantly the original model while yet preserving its original structure to the extent possible. They formally stated two problems: calculating the smallest objective subset that preserves the dominance structure considering a fixed approximation error; and computing the minimum error for a subset of objectives of given size. The same authors proposed two algorithms to solve these problems, one exhaustive and another one heuristic. More recently, Guillén-Gosálbez²⁹ proposed an alternative MILPbased method to solve both problems 19 that takes advantage of the latest branch-and-cut methods developed for MILP.

In this work, we optimize utility plants under different environmental metrics and study the relationships between environmental indicators using a rigorous dimensionality reduction strategy. The approach presented relies on the combined use of multiobjective optimization, LCA analysis and dimensionality reduction methods. The planning task is first posed as a multiobjective mixed-integer linear problem (MILP) that simultaneously accounts for the minimization of the cost and environmental impact of the energy system. The

environmental performance of the system is modeled using several LCA-based indicators that quantify the damage caused in different categories. A dimensionality reduction technique is then applied to facilitate the postoptimal analysis of the solutions found.

The paper is organized as follows. Section 2 presents a formal definition of the problem under study. In section 3, the mathematical formulation derived to address this problem is presented. Section 4 describes the solution strategy employed to solve the MILP model, paying special attention to the dimensionality reduction strategy. In section 5, the capabilities of the proposed modeling framework and solution strategy are illustrated through two case studies, while in section 6 the conclusions of the work are drawn.

2. PROBLEM STATEMENT

The problem to solve can be formally stated as follows. We are given the electricity and steam demand at various pressure levels to be satisfied, environmental data associated with the production and combustion of fuels, and electricity generation and process data. The goal of the analysis is to determine the set of planning decisions that simultaneously minimize the total cost and the associated environmental impact. Decisions to be made include the amounts and types of fuels to be burnt in the boilers and turbines of the system, along with the amount of electricity purchased from an external supplier. The optimization model presented in section 3 includes empirical models for tanks, boilers, and mixers that reproduce the behavior of a standard utility plant.

3. MATHEMATICAL FORMULATION

Energy systems utilize fuel, air, and other materials to generate electricity and steam demanded by other process units of an industrial system (see Figure 1). The system taken as reference in this work consists of storage tanks to store a set of fuels, boilers that convert fuels into steam at high pressure, and turbines that expand higher pressure steam into lower pressure steam in order to generate electricity.

The flows of materials in the units are denoted by the continuous variables $x_{jltm}^{\rm FU}$ (fuel); $x_{jlt}^{\rm HP}$, $x_{jlt}^{\rm MP}$, and $x_{jlt}^{\rm LP}$ (steam at high, medium, and low pressure, respectively); $x_{jlt}^{\rm CO}$ (condensate); and $x_{jlt}^{\rm EL}$ (electricity). In these variables, the subscript j represents the process unit of the system to which the flow is referred (i.e., tanks, boilers, or turbines), l denotes the state of the material (i.e., input or output), and t indicates the time period (as discussed later in the paper, the examples addressed herein consider seven time periods with 48 h each). There may be different types of fuel available in the system, which are denoted by index m (fuels 1-4).

The overall problem is formulated using the generalized disjunctive programming (GDP) framework that integrates the

discrete and continuous decisions to be made in the system effectively using Boolean and continuous variables. In the GDP problem, logic decisions correspond to the selection of a specific fuel type among a set of available choices. The complete formulation is described in detail in sections 3.1–3.5.

3.1. Fuel Tank Models. Fuel tanks may use different fuels that are combusted in the boilers in order to generate high pressure (HP) steam. There are several reasons for considering alternative fuels instead of a single one. One of them is the lack of a certain fuel type due to problems in the supply in a given time period. Another possible reason is the inclusion of economically and/or environmentally attractive fuels in order to improve the economic performance of the system and/or minimize its environmental impact. Specifically, the selection of a specific fuel m in a tank j in period t can be modeled with the following disjunction:

$$\begin{aligned} & \text{TFC}_{jt} = \text{cost}_{mt}^{\text{FU}} x_{jltm}^{\text{FU}} \theta \\ & \text{TIC}_{jt} = \text{cost}_{mt}^{\text{INV}} \left(\frac{\text{INV}_{jt-1m} + \text{INV}_{jtm}}{2} \right) \\ & \text{INV}_{jtm} = \text{INV}_{jt-1m} + \theta (x_{jltm}^{\text{FU}} - x_{jl'tm}^{\text{FU}}) \\ & \frac{x_{jt}^{\text{FU}}}{2} \leq x_{jl''tm}^{\text{FU}} \leq \overline{x_{jt}^{\text{FU}}} \\ & \text{INV}_{jt} \leq \text{INV}_{jtm} \leq \overline{\text{INV}_{jt}} \end{aligned}$$

 $\forall t, j \in TANKS, l = IN, l' = OUT, l'' = IN, OUT$

$$Y_{jtm} \in \{\text{True, False}\} \quad \forall m, t, j \in \text{TANKS}$$
 (1)

If fuel m is stored in tank j in period t, then the Boolean variable Y_{jtm} will be True, and the total fuel cost (TFC $_{jt}$), the inventory level in the tank (INV $_{jtm}$), and the associated inventory cost (TIC $_{jt}$) will take positive values that will be defined by specific equations. The remaining terms of the disjunction, which correspond to the other fuels (i.e., $m \neq m$), will be inactive (i.e., $Y_{jtm} = \text{False}$), and hence, all their constraints will be ignored and the associated variables will be set to zero.

For the selected fuel, the total fuel cost (TFC_{it}) is calculated from the fuel consumption and the fuel cost in period t (cost FU). Here, θ represents the duration of each period t. The inventory level in the tank is given by the material balance, which states that the final inventory (INV_{itm}) must be equal to the initial inventory (INV $_{jt-1m}$) plus the amount of fuel introduced in the tank minus the amount transferred from the tank to the boilers. The total inventory cost (TIC_{it}) is calculated from the average inventory in period t and the unit inventory cost associated with fuel m ($\cos \tilde{t}_{mt}^{\mathrm{INV}}$). The disjunction enforces also lower and upper limits on the mass flows and inventory levels of the fuels $(\underline{x_{jt}^{FU}}, \underline{INV_{jt}}, \underline{x_{jt}^{FU}}, \underline{and} \underline{INV_{jt}})$ respectively), provided the corresponding fuel is selected. All these variables are calculated only when the associated Boolean variable is True, and they are set to zero otherwise. Note that, for the first time period (t = 1), variable INV_{it-1m} appearing in the disjunction must be replaced by the parameter INVini, m, which denotes the initial inventory of fuel m in tank j.

3.2. Boiler Models. Boilers generate high pressure steam by burning fuel. The combustion process generates environmentally harmful chemical substances such as SO_x, NO_x, and

 CO_x . These units require electricity for operating the mechanical equipment and medium pressure steam for heating the boiler feedwater. Similarly, as with the tanks, boilers can utilize different fuels with some adjustments in the operating conditions of their equipment. The boilers are modeled with the following disjunctions:

$$\begin{bmatrix} Y_{jtm} \\ x_{jlt}^{\text{HP}} = \frac{hc_m}{\eta_{jm}} x_{jl'tm}^{\text{FU}} \\ \\ x_{jt}^{\text{FU}} \leq x_{jl'tm}^{\text{FU}} \leq \overline{x_{jt}^{\text{FU}}} \end{bmatrix}$$

 $\forall t, j \in BOILERS, l = GEN, l' = CON$

$$Y_{jtm} \in \{\text{True, False}\} \quad \forall m, t, j \in \text{BOILERS}$$
 (2)

When a given fuel m is selected, the corresponding term of the disjunction is active (i.e., Y_{jtm} is True), and the amount of HP steam is calculated from the amount of fuel consumed, the heat of combustion of the selected fuel (hc_m), and the boiler efficiency (η_{jm}). Besides, lower and upper bounds are enforced on the total fuel consumption. On the other hand, if a fuel m is not selected, the corresponding term of the disjunction is inactive (i.e., Y_{jtm} is False) and the fuel consumption in the boiler and the amount of steam generated are both set to zero.

The amount of medium pressure (MP) steam and electricity consumed in a boiler are a function of the HP generated, as stated in eqs 3 and 4.

$$x_{jlt}^{\text{MP}} = a_j^{\text{MP}} x_{jl't}^{\text{HP}} \quad \forall t, j \in \text{BOILERS}, l = \text{CON}, l'$$

$$= \text{GEN}$$
(3)

$$x_{jlt}^{\text{EL}} = a_j^{\text{EL}} x_{jl't}^{\text{HP}} \quad \forall t, j \in \text{BOILERS}, l = \text{CON}, l'$$

$$= \text{GEN}$$
(4)

In eqs 3 and 4, $a_j^{\rm MP}$ and $a_j^{\rm EL}$ represent the materials balance coefficients that relate the amount of HP steam generated in boiler j with the consumption of MP steam and electricity.

The total amount of fuel consumed in the boilers must be equal to the amount sent from the storage tanks:

$$\sum_{j \in \text{BOILERS}} x_{jltm}^{\text{FU}} = \sum_{j \in \text{TANKS}} x_{jl'tm}^{\text{FU}}$$

$$\forall t, m, l = \text{CON}, l' = \text{OUT}$$
(5)

Note that eqs 3-5 must be satisfied regardless of the fuel selected, and hence can be placed outside the disjunction.

3.3. Turbine Models. Turbines expand steam at higher pressure by converting the mechanical energy released during the expansion into electricity. A typical multistage turbine receives HP steam and produces electricity, MP and low pressure (LP) steams and condensate, as shown in Figure 1. Electricity generation in a turbine is a function of the amount of HP steam feed, the amounts of MP and LP steam, and the amount of condensate generated, as shown in eq 6.

$$\begin{aligned} x_{jlt}^{\text{EL}} &= b_{j}^{\text{HP}} x_{jl't}^{\text{HP}} - g_{j}^{\text{MP}} x_{jlt}^{\text{MP}} - g_{j}^{\text{LP}} x_{jlt}^{\text{LP}} - g_{j}^{\text{CO}} x_{jlt}^{\text{CO}} \\ \forall t, j \in \text{TURBINES}, l = \text{GEN}, l' = \text{IN} \end{aligned} \tag{6}$$

In eq 6, the coefficients $b_j^{\rm HP}$, $g_j^{\rm MP}$, $g_j^{\rm LP}$, and $g_j^{\rm CO}$ can be obtained by performing a statistical analysis on the existing process data.

The upper and lower bounds on the amount of electricity generated in turbines are defined via eq 7.

$$\underline{x_{jlt}^{\text{EL}}} \le x_{jlt}^{\text{EL}} \le \overline{x_{jlt}^{\text{EL}}} \qquad \forall \ j \in \text{TURBINES}, \ t, \ l = \text{GEN}$$
(7)

The material balance around turbines is expressed in eq 8:

$$x_{jlt}^{HP} = x_{jl't}^{MP} + x_{jl't}^{LP} + x_{jl't}^{CO}$$

$$\forall t, j \in \text{TURBINES}, l = \text{IN}, l' = \text{GEN}$$
(8)

3.4. Demand Satisfaction. The demands of electricity, HP, MP, and LP steam must be fulfilled in each time period, as stated in constraints 9-12:

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{EL}} + \text{EPU}_t - \sum_{j \in \text{BOILERS}} \sum_{l = \text{CON}} \theta x_{jlt}^{\text{EL}}$$

$$\geq \text{dem}_t^{\text{EL}} \quad \forall t$$
(9)

$$\sum_{j \in \text{BOILERS}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{HP}} - \sum_{j \in \text{TURBINES}} \sum_{l = \text{IN}} \theta x_{jlt}^{\text{HP}} \ge \text{dem}_t^{\text{HP}}$$

$$\forall t$$
 (10)

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{MP}} - \sum_{j \in \text{BOILERS}} \sum_{l = \text{CON}} \theta x_{jlt}^{\text{MP}} \ge \text{dem}_t^{\text{MP}}$$

$$\forall t$$
 (11)

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{LP}} \ge \text{dem}_t^{\text{LP}} \qquad \forall \ t$$
(12)

Here dem_t^{EL} , dem_t^{HP} , dem_t^{MP} , and dem_t^{LP} denote the demands of electricity and HP, MP, and LP steam in period t, whereas EPU $_t$ represents the total amount of electricity purchased from the external supplier. Hence, eq 9 considers that part of the electricity demand can be satisfied by an external supplier (i.e., outsourcing). Note that, in eq 10, the amount of HP steam available is calculated from the steam generated in the boiler minus the amount consumed in the turbine. Similarly, in eq 11, the total amount of MP steam available is obtained by subtracting the consumption of steam in the boiler from the amount of MP steam produced in the turbine.

- **3.5. Objective Functions.** The model presented must attain two targets: minimum cost and environmental impact. We next describe in detail how to determine both objectives.
- 3.5.1. Total Cost. The total cost (TC) of the energy system includes the cost of the fuel purchased, the inventory cost associated with holding fuel in the tanks, and the consumption of external electricity, as stated in eq 13:

$$TC = \sum_{j \in TANKS} \sum_{t} TFC_{jt} + \sum_{j \in TANKS} \sum_{t} TIC_{jt} + \sum_{t} cost_{t}^{EL} EPU_{t}$$
(13)

Here, $cost_t^{EL}$ is the electricity cost in period t.

3.5.2. Environmental Impact Objective Function. The environmental performance of the energy system is quantified according to the principles of life cycle assessment (LCA).³⁰ Specifically, this work makes use of the Eco-indicator 99 framework, which accounts for 11 impacts aggregated into three damage categories. The computation of this metric follows the four LCA phases: goal and scope definition,

inventory analysis, impact assessment, and interpretation. Such phases are described in detail in sections 3.5.2.1–3.5.2.4.

- 3.5.2.1. Goal and Scope Definition. In this phase, the system boundaries and the impact categories are identified. Specifically, a "cradle-to-grave" analysis is carried out, which embraces all the activities of the energy system, starting from the extraction of raw materials (i.e., oil), and ending with the delivery of electricity and steam to the final customers. Eleven impact categories, as defined by the Eco-indicator 99, are considered:
 - 1. carcinogenic effects on humans
 - respiratory effects on humans caused by organic substances
 - respiratory effects on humans caused by inorganic substances
 - 4. damage to human health caused by climate change
 - 5. human health effects caused by ionizing radiations
 - 6. human health effects caused by ozone layer depletion
 - damage to ecosystem quality caused by ecosystem toxic emissions
 - 8. damage to ecosystem quality caused by the combined effect of acidification and eutrophication
 - 9. damage to ecosystem quality caused by land occupation and land conversion
- 10. damage to resources caused by extraction of minerals
- 11. damage to resources caused by extraction of fossil fuels
- 3.2.2.2. Inventory Analysis. The second phase of the LCA provides the inputs and outputs of materials and energy associated with the process (life cycle inventory), which are required to perform the environmental impact calculations. In the context of the energy system, the environmental burdens are given by the production of fuels at the refineries (LCI_b^{FU}), the generation of the external electricity (LCI_b^{EL}), and the direct emissions associated with the combustion of the fuels in the boilers (LCI_b^{DE}). Mathematically, the inventory of emissions can be expressed as a function of some continuous decision variables of the model, as stated in eq 14.

$$\begin{split} & \operatorname{LCI}_{b} = \operatorname{LCI}_{b}^{\operatorname{FU}} + \operatorname{LCI}_{b}^{\operatorname{EL}} + \operatorname{LCI}_{b}^{\operatorname{DE}} \\ & = \sum_{j \in \operatorname{TANKS}} \sum_{l = \operatorname{IN}} \sum_{t} \sum_{m} \theta \omega_{mb}^{\operatorname{FU}} x_{jltm}^{\operatorname{FU}} + \sum_{t} \omega_{b}^{\operatorname{EL}} \operatorname{EPU}_{t} \\ & + \sum_{j \in \operatorname{BOILERS}} \sum_{l = \operatorname{CON}} \sum_{t} \sum_{m} \theta \omega_{mb}^{\operatorname{DE}} x_{jltm}^{\operatorname{FU}} \quad \forall \ b \end{split}$$

Here, $\omega_{mb}^{\rm FU}$, $\omega_b^{\rm EL}$, and $\omega_{mb}^{\rm DE}$ denote the life cycle inventory entries (i.e., feedstock requirements and emissions released) associated with chemical b per reference flow of activity. In the production of fuels and electricity, the reference flow is one unit of fuel (tons) and electricity (kW), respectively, generated. In the combustion of fuel, the reference flow is one unit of fuel combusted in the boilers.

3.5.2.3. Impact Assessment. In this step, the environmental impact of the process is determined using a damage assessment model. These impacts are further aggregated into three main damage categories: human health (expressed in disability-adjusted life years (DALYs)), ecosystem quality (potentially disappeared fraction (PDF)·m²·year)), and damages to resources (megajoules (MJ) surplus energy). Mathematically, the damage caused in impact category c belonging to damage category d (IM $_c$) is calculated from the life cycle inventory and a set of damage factors (df $_{bc}$), as stated in eq 15.

$$IM_c = \sum_b df_{bc} LCI_b \qquad \forall c$$
(15)

The damage factors link the LCI results to the damage in each impact category. There are three different damage models, each of which reflects a different perspective based on cultural theory.³¹ The impact caused in each damage category can be calculated via eq 16:

$$DAM_d = \sum_{c \in ID(d)} IM_c \qquad \forall d$$
(16)

Here, ID(d) denotes the set of impact categories c that contribute to damage d. Finally, the damages are normalized and aggregated into a single impact factor (i.e., Eco-indicator 99), as stated in eq 17.

$$ECO_{99} = \sum_{d} n_d w_d DAM_d \tag{17}$$

This equation makes use of normalization (n_d) and weighting (w_d) factors, whose values are specified in the Eco-indicator 99 methodology.³¹

3.5.2.4. Interpretation. Finally, in the fourth phase, the results are analyzed and a set of conclusions or recommendations is formulated. In our work, the preferences of decision-makers are articulated in the postoptimal analysis of the Pareto optimal solutions.

4. SOLUTION STRATEGY

The overall multicriteria GDP can be expressed as follows:

$$\min Z = (TC, EI_1, EI_2, ..., EI_{11})$$

$$\bigvee_{i} \begin{bmatrix} Y_{i} \\ h_{j}(x) \leq 0 \\ c_{j} = \gamma_{j} \end{bmatrix}$$

$$\Omega(Y) = TRUE$$

$$x \ge 0$$
 $c_i \ge 0$ $Y_i \in \{\text{True, False}\}$

Where EI_1 to EI_{11} represent the impacts in the different categories. Using the convex hull reformulation technique, ³² the GDP is reformulated into a multicriteria mixed-integer linear programming (MILP) model of the following type:

(MO)

$$\min_{x,y}(TC, EI_1, EI_2, ..., EI_{11})$$

s.t.

$$g(x, y) \leq 0$$

$$h(x, y) = 0$$

$$x \in \mathbb{R}$$
, $v \in \{0, 1\}$

in which TC represents the total cost, EI is the LCA impact in every category, x denotes the continuous variables (mass flows, inventory levels, and costs), and y represents the binary variables that replace the Boolean variables of the GDP problem. This model contains a large number of objectives, so the direct application of standard multiobjective optimization methods such as the epsilon constraint or weighted sum might lead to very large CPU times. In this paper, this model is solved

by an approximation strategy that comprises three steps. In step I, a set of Pareto points are generated using an heuristic approach that decomposes the model into a set of bicriteria problems. In step II, a dimensionality reduction algorithm is applied to identify redundant objectives that can be eliminated from the analysis while still keeping the problem structure to the extent possible. In step III, the model is optimized again but this time in a reduced domain of objectives. The steps can be applied iteratively until a desired number of Pareto solutions is generated.

4.1. Step I: Generation of an Initial Set of Pareto Solutions. A set of solutions of the original multiobjective model are first generated using a heuristic-based approach³³ that decomposes the original problem into a set of bicriteria subproblems in each of which the cost is optimized against each single impact separately. Hence, a series of bicriteria models of the following form are calculated:

(MO)

$$\min_{x,y}(\text{TC, EI})$$
s.t.

$$g(x, y) \le 0$$

$$h(x, y) = 0$$

$$x \in \mathbb{R}, \quad y \in \{0, 1\}$$

where EI represents here the specific impact being optimized in every subproblem. Note that solving these bicriteria problems takes much less time than solving the original model in its original domain. This is because multiobjective optimization problems are very sensitive to the number of objectives. Without loss of generality, the epsilon constraint³⁴ is employed to solve the bicriteria subproblems. This method solves a set of single objective problems, in each of which one objective is optimized and the other is transferred to an auxiliary constraint that bounds it within some allowable levels.

The Pareto solutions generated in this manner are next normalized, and finally used to carry out an MILP-based dimensionality reduction analysis that identifies redundant objectives that can be omitted without disturbing significantly the main features of the problem.

We then normalize the Pareto solutions by dividing each objective function value by the maximum value attained by the objective in all of the solutions.

4.2. Step II: Postoptimal Analysis: Dimensionality Reduction Methods. After normalizing the solutions, we apply a dimensionality reduction method based on the work by Guillén-Gosálbez.²⁹ Dimensionality reduction methods eliminate redundant objectives from the model, thereby facilitating the generation and postoptimal analysis of the Pareto solutions.

A simple example is used to illustrate the manner in which dimensionality reduction works. The concept of weakly Pareto efficiency is considered throughout the paper. A solution A is called weakly efficient if there are no other solutions that are strictly better than A simultaneously in all of the objectives. Let us now consider four weakly efficient solutions of a multiobjective problem (solutions A, B, C, and D) that optimize four objective functions $F = f_1, f_2, f_3, f_4$ (i.e., we aim to minimize all of them simultaneously). Figure 2 is a parallel coordinates plot which shows in the bottom axis the different objective functions and in the vertical axis the normalized

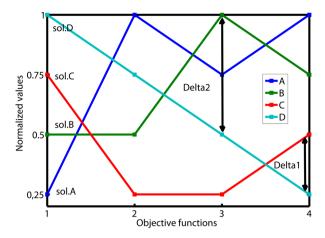


Figure 2. Dominance structure for the set f_1 , f_2 , f_3 , f_4 . All solutions are weakly efficient because no one dominates any of the others; that is, there is no solution with better performance simultaneously in all of the objectives than any of the other points.

values attained by each solution in every objective. As seen, the four solutions are weakly Pareto efficient, as none of them improves any of the others simultaneously in all of the objectives. Because the solutions are Pareto optimal, their corresponding lines in the parallel coordinates plot intersect in at least one point.

Let us now assume that we remove one objective from the search space, let us say objective f_4 . Figure 3 depicts the

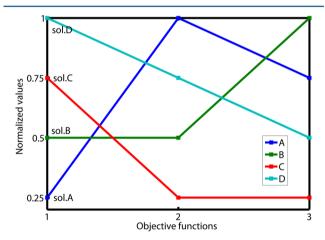


Figure 3. Dominance structure for the reduced set f_1 , f_2 , f_3 . Solution C dominates solution D, since C is better than D in all the objectives. Solution D is therefore lost. A delta error then is generated, which is the maximum value we have to subtract from the solution lost so that it is optimal in the reduced domain (see Figure 2).

dominance structure of the reduced space $F' = f_1$, f_2 , f_3 . It can be seen that now solution C dominates solution D in the reduced space, since C is better than D in all of the objectives kept. Hence, removing f_4 changes the dominance structure of the problem, as solution D becomes suboptimal in the reduced space F'.

Brockhoff and Zitzler²⁶ proposed a metric to quantify the extent to which the initial dominance structure of a problem changes after removing objectives. This metric, termed "delta error", corresponds to the difference between the true value of objective f_4 in solution C and the value required to dominate solution D in the original space of objectives (see Figure 2). In

our example, the reduced objective set, $F' = f_1$, f_2 , f_3 , could replace the original set, $F = f_1$, f_2 , f_3 , f_4 , incurring in a delta error of 0.25.

If two objectives, say f_4 and f_3 , are omitted, then solution D becomes dominated by solutions C and B (see Figure 4). In

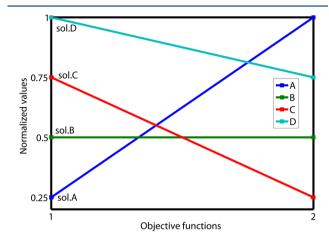


Figure 4. Dominance structure for the reduced set f_1 , f_2 . Solution C and B dominate solution D, since C and B are better than D in all objectives. Solution D is therefore lost, and a delta error is generated (see Figure 2).

this case, the delta error is 0.5, which corresponds to the maximum value that we have to subtract to the solutions lost so as to be dominated in the original objectives space (and not only in the reduced objectives space) (see Figure 2). Hence, it is clear that higher delta values imply greater changes in the dominance structure of the problem.

Note that the delta value depends on the objectives removed. As an example, discarding the second and third objectives (reduced space $F''' = f_1$, f_4) produces no changes in the dominance structure, since all the solutions are kept (see Figure 5). In this case, we say that the reduced objective set $F''' = f_1$, f_4 is nonconflicting with the original one $F = f_1$, f_2 , f_3 , f_4 . That implies that F''' can be replaced by F without changing the dominance structure of the problem (delta error = 0). The goal

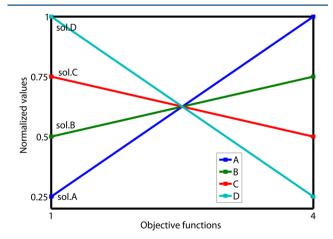


Figure 5. Dominance structure for reduced set f_1 , f_4 . No solution dominates any of the others. All solutions are Pareto optimal in the reduced search space, and the dominance structure is preserved. By selecting the objectives to be dominated in a smart manner, it is possible to reduce the dimension of the problem while still preserving fully its structure.

of dimensionality reduction methods is therefore to identify objectives that can be removed with a minimum change in the dominance structure of the problem (i.e., minimum delta error).

An MILP-based dimensionality reduction method introduced by Guillén-Gosálbez²⁹ is applied in this work to conduct the dimensionality-reduction analysis described above. This method identifies redundant objectives that can be omitted at minimum delta error. Further details on this strategy can be found elsewhere.^{19,29,35,36}

- **4.3. Step III: Solution of the Multiobjective Model in the Reduced Domain.** After identifying the redundant objectives, the original model is next solved but this time in the reduced space. Step II can then be repeated by applying the dimensionality reduction algorithm again but this time taking more Pareto points as input data in an attempt to reduce further the dimension of the model.
- **4.4. Remarks.** Regarding the solution strategy and steps I—III:
- 1. The bicriteria problems solved in step I can be calculated with any standard multiobjective optimization algorithm.
- 2. Numerical results show that the dimensionality reduction algorithm is capable of identifying redundant objectives even using a small number of Pareto points. Because of this, a single run of the three steps (see sections 4.1, 4.2, and 4.3) suffice to generate good results for the problem.
- 3. The overall method includes some tuning parameters, such as the number of Pareto points generated in each bicriteria problem as well as in the reduced model solved in step III. In addition, a maximum delta error needs to be specified in the dimensionality reduction MILP.
- 4. In addition to expediting the generation of Pareto solutions, our approach provides valuable insight into the relationships between the economic and environmental indicators of concern for decision-makers.

5. CASE STUDY

The capabilities of our modeling framework and solution strategy are illustrated using two case studies that address the optimal planning of an energy system with two fuel tanks, two boilers, and two turbines (see Figure 6). Both case studies assume the same data concerning fuel types, equipment units, and energy demands, but differ in the characteristics of the electricity purchased. A total of 13 objectives are included (i.e., total cost, the 11 Eco-indicator 99 impacts, and the total Eco-indicator 99). Data retrieved from environmental databases³⁷ is employed in the calculations. The motivation for optimizing the Eco-indicator 99 along with its single impacts is to analyze whether the minimization of an aggregated impact is a good practice when optimizing utility systems (i.e., it preserves the problem structure). As will be shown next, the suitability of the Eco-indicator 99 depends on the problem characteristics.

The initial demand of electricity is 29 MW for both examples. The initial demand of steam (HP, MP, and LP) is 2, 92, and 98 tons/h, respectively. A 5% increase in this demand is defined for each period. The model covers seven time periods with 48 h each. Fuel data are given in Table 1. The parameters associated with boilers are displayed in Tables 2 and 3. The parameters of the turbines are given in Table 4. The capacity of tanks 1 and 2 are 120 and 50 tons, respectively. The maximum electricity power provided by each turbine is 70 MW. The LCA data associated with the production of the different fuels are presented in Table 5, and the impacts associated with the

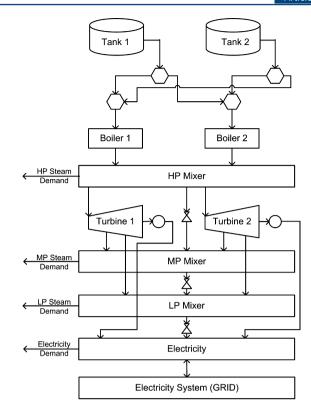


Figure 6. Superstructure of case study.

Table 1. Data for Fuels: Heat of Combustion (hc_m), Greenhouse Gas Content (ghg_m), Price ($cost_{mt}^{FU}$), and Inventory Cost ($cost_{mt}^{INV}$)

fuel	$hc_m (kJ/ton)$	ghg_m (kg/ton)	$cost_{mt}^{FU}$ (\$/ton)	$cost_{mt}^{INV}$ (\$/ton·h)
1	10.50	17	200	0.50
2	9.65	5	76	0.19
3	6.65	3	83	0.20
4	10.20	10	145	0.35

Table 2. Data for Boilers: I. Boiler Efficiency (η_{im})

	η_{jm} (kJ/ton)				
fuel	boiler 1	boiler 2			
1	0.59	0.58			
2	0.60	0.60			
3	0.56	0.57			
4	0.61	0.60			

Table 3. Data for Boilers: II. Materials Balance Coefficients $(a_i^{\text{MP}} \text{ and } a_i^{\text{EL}})$

boiler	a_j^{MP} (ton/ton)	$a_j^{\rm EL}$ (ton/MW·h)
1	0.11	0.002
2	0.12	0.003

external electricity are displayed in Table 6. The parameters of the damage model were taken from the Eco-indicator 99 report,³¹ assuming the average weighting set and the hierarchic perspective.

Numerical experiments were carried out in the modeling system GAMS. The number of variables and constraints varies according to the instance being solved. The standard MILP formulation contains 667–753 continuous variables, 112 binary variables, and 765–852 equations. The MILPs were solved with

Table 4. Data for Turbines: Materials Balance Coefficients $(g_i^{LP}, g_i^{MP}, g_i^{HP},$ and $g_i^{CO})$

turbine	g_j^{LP} (MW·h/ton)	g_j^{MP} (MW·h/ton)	$g_j^{\rm HP}$ (MW·h/ton)	g_j^{CO} (MW·h/ton)
1	0.01	0.07	0.15	0.00
2	0.01	0.08	0.18	0.00

Table 5. Environmental Data: Production of Fuels

	fuel (impact/kg)				
	1	2	3	4	
carcinogens (DALYs)	1.05×10^{-8}	1.27×10^{-8}	1.29×10^{-8}	2.52×10^{-9}	
respiratory effects (org) (DALYs)	1.64×10^{-9}	1.69×10^{-9}	1.90×10^{-9}	1.00×10^{-11}	
respiratory effects (inorg) (DALYs)	3.81×10^{-7}	4.36×10^{-7}	4.54×10^{-7}	8.23×10^{-9}	
climate change (DALYs)	7.18×10^{-8}	8.73×10^{-8}	8.85×10^{-8}	1.92×10^{-9}	
ionizing radiation (DALYs)	7.70×10^{-10}	9.10×10^{-10}	9.40×10^{-10}	2.00×10^{-11}	
ozone layer depletion (DALYs)	4.70×10^{-10}	4.80×10^{-10}	5.40×10^{-10}	0.00	
ecotoxicity (PDF·m²·year)	4.71×10^{-2}	6.08×10^{-2}	5.88×10^{-3}	8.15×10^{-4}	
acidif/eutroph (PDF·m²·year)	1.05×10^{-2}	1.21×10^{-2}	1.25×10^{-2}	2.96×10^{-4}	
land use (PDF·m²-year)	1.27×10^{-4}	1.44×10^{-4}	1.52×10^{-4}	1.32×10^{-4}	
minerals extraction (MJ)	3.09×10^{-5}	2.50×10^{-5}	2.05×10^{-5}	2.99×10^{-7}	
fossil fuels extraction (MJ)	6.92	7.07	8.02	8.38×10^{-3}	

Table 6. Environmental Data: Generation of Electricity

	electricity		
	example 1 (impact/MJ)	example 2 (impact/kWh)	
carcinogens (DALYs)	1.66×10^{-8}	1.06×10^{-8}	
respiratory effects (org) (DALYs)	7.00×10^{-11}	7.30×10^{-9}	
respiratory effects (inorg) (DALYs)	1.58×10^{-7}	7.30×10^{-9}	
climate change (DALYs)	3.15×10^{-8}	2.36×10^{-9}	
ionizing radiation (DALYs)	4.72×10^{-9}	4.12×10^{-11}	
ozone layer depletion (DALYs)	5.00×10^{-11}	6.44×10^{-13}	
ecotoxicity (PDF·m²·year)	2.12×10^{-3}	1.80×10^{-4}	
acidif/eutroph (PDF·m²·year)	3.57×10^{-3}	3.68×10^{-3}	
land use (PDF·m²-year)	6.05×10^{-3}	7.11×10^{-4}	
minerals extraction (MJ)	2.43×10^{-4}	5.93×10^{-3}	
fossil fuels extraction (MJ)	5.20×10^{-2}	5.38×10^{-3}	

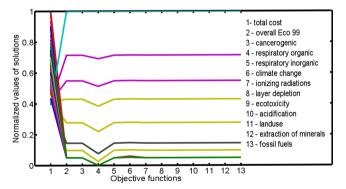


Figure 7. Parallel coordinate plot for example 1. We show in the horizontal axis the different objectives, and in the vertical one the normalized value of each solution in each objective. Normalization is performed by subtracting the minimum value for each objective function value and dividing by the difference between the maximum and the minimum attained over all the solutions.

the solver CPLEX on a 2x AMD Athlon 2.99 GHz processor, with 3.49 GB of RAM. It took around 0.1–0.4 CPU s to solve each MILP.

5.1. Example 1. This example considers an external electricity provider (i.e., electricity mix) with a high environ-

mental impact (see Table 6) and low price (\$2/MWh). A total of 240 Pareto solutions were generated by optimizing each environmental criterion vs the total cost. Figure 7 is a parallel coordinates plot that depicts in the horizontal axis the different objective functions, and in the vertical axis the normalized value attained by each solution in every objective. The normalization is performed by dividing each objective value by the maximum one attained over all of the solutions. As observed, the environmental objectives seem to be equivalent, since when one objective increases so do the others and vice versa. Hence, the cost (on the one hand) and the environmental impacts (on the other) behave in opposite manners; that is, reductions in the first result in increments in the second ones and vice versa.

Figure 8 shows the normalized results. The horizontal axis shows the normalized total cost, while the vertical one shows the normalized environmental impacts. Figure 8 depicts all the solutions in the two-dimensional space (Eco-indicator 99, cost). The blue squares represent the solutions obtained when optimizing the Eco-indicator 99 against the cost, while the red circles are the solutions resulting from the optimization of the total cost against each single impact category. As observed, the optimization of the Eco-indicator 99 produces solutions that are quite close to those obtained when optimizing each impact category separately. This observation is therefore consistent with the analysis of the parallel coordinates plot, which suggested that all the indicators behave similarly.

It is noteworthy that every solution implies a different combination of fuel and electricity (see Table 7). For example, in solution A (i.e., minimum cost solution in Figure 8), a fraction of the electricity demand is met by purchasing it from an external supplier, whereas the remaining demand is generated from fuel 2. In solution B, a significant portion of electricity is generated from fuel 2, whereas in solution C electricity is mainly generated from fuel 3. The reason why all of the environmental impacts behave similarly and the cost is conflictive with them is that the cost depends to a large extent on the amount of fuel purchased, while the environmental metrics depend largely on the electricity consumption.

Figure 8 provides some interesting insight into this problem. As seen, the Pareto curve Eco-indicator 99 vs cost (blue circles in Figure 8) is rather smooth in the region that goes from B to

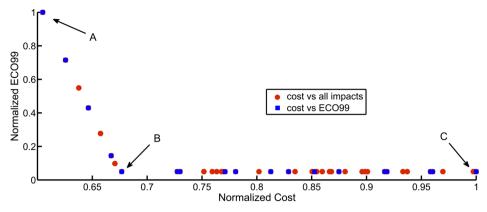


Figure 8. Results obtained from the bicriteria problem cost vs the overall Eco-indicator 99 (blue points) and from solving the bicriteria problems cost vs single impacts (red points) for example 1.

Table 7. Consumption of Fuel and External Electricity in Different Solutions (See Figure 8) for Example 1

soln	purchased electricity (MW)	fuel 1 (tons)	fuel 2 (tons)	fuel 3 (tons)	fuel 4 (tons)
A	2498.88	0	4626.61	0	0
В	673.36	0	5233.41	0	0
C	673.36	0	0	7088.05	0

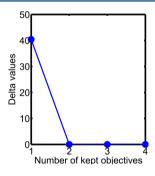


Figure 9. Minimum of delta value for different sets of number of objectives. Example 1.

Table 8. Delta Values for Example 1 for All Combinations of Two Objectives a

redu	ced set	
		delta
1	2	0.0081
1	3	0.2602
1	4	0.2602
1	5	0.2602
1	6	0.0031
1	7	0.2602
1	8	0.2602
1	9	0.1516
1	10	0.2602
1	11	0.2602
1	12	0.2602
1	13	0.2602

"Here 1 is total cost, and other objectives are environmental impacts: 2 is overall ECO₉₉, 3 is carcinogenic, 4 is respiratory organic, 5 is respiratory inorganic, 6 is climate change, 7 is ionizing radiation, 8 is layer depletion, 9 is ecotoxicity, 10 is acidification, 11 is land use, 12 is extraction of minerals, and 13 is fossil fuels.

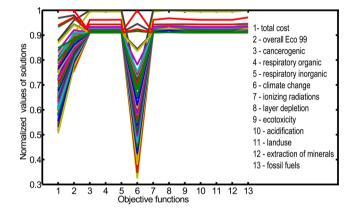


Figure 10. Parallel coordinate plot for example 2.

C, whereas in the region that goes from A to B increases sharply (when the model decides to increase the amount of electricity purchased from outside).

The MILP for dimensionality reduction ^{19,29} is run next to analyze the relationships between different environmental indicators. Figure 9 shows the minimum delta value for different numbers of objectives kept. As observed, the delta error diminishes with the number of objectives retained. From one to two, this drop is quite significant, while afterward (as we increase further the number of objectives kept) is close to zero and flat. This is because, as mentioned before, all the impacts behave similarly and one of them is enough to capture the behavior of the remaining ones.

Table 8 shows the delta value corresponding to every possible combination of cost vs each single environmental impact. All combinations of cost and impact yield a very small approximation error (delta value). Hence, the original multi-objective problem could be approximated by one bicriteria model (which would optimize the cost against any of the single environmental indicators) without significant changes in the problem structure.

5.2. Example 2. An external electricity source at high price (\$243/MWh) and a low environmental impact are considered in this example (see Table 6). The electricity is assumed to be generated by wind energy. A total of 240 Pareto solutions are calculated by optimizing each environmental objective vs the total cost.

Figure 10 presents the normalized values for every objective in a parallel coordinates plot. As observed, some objectives behave in a conflictive manner. Particularly climate change is

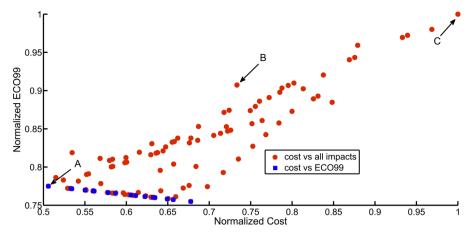


Figure 11. Points resulting from the bicriteria optimization cost vs Eco-indicator 99 and cost vs every single impact projected onto the subspace cost vs Eco-indicator 99. Red points above the envelope of the blue ones would be lost if Eco-indicator 99 and cost were optimized as unique objectives (example 2).

Table 9. Consumption of Fuel and External Electricity in Different Solutions (See Figure 11) for Example 2

soln	purchased electricity (MW)	fuel 1 (tons)	fuel 2 (tons)	fuel 3 (tons)	fuel 4 (tons)
A	673.36	0	5233.41	0	0
В	736.17	0	2511.72	0	3062.082
C	673.36	4729.59	0	0	0

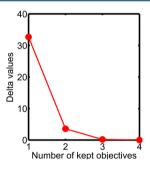


Figure 12. Minimum of delta value for different sets of kept objectives. Example 2.

conflicting with other objectives, since solutions with low climate change impact show large impacts in other categories and vice versa. As will be explained later, these conflicts arise when the same decision variable has opposite contributions in different environmental impacts.

In Figure 11, the bottom axis shows the normalized total cost and the vertical one the normalized Eco-indicator 99. The blue points are the solutions to the bicriteria problem Eco-indicator 99 vs total cost, while red points represent the solutions of the bicriteria problems (total cost vs each single impact category separately). As opposed to the previous example, it happens now that some solutions would be discarded if cost and Eco-indicator 99 were the only objectives minimized. This is because some solutions that are optimal in the space of individual objectives (when optimizing some individual objectives vs the total cost) are suboptimal in the space (Eco-indicator 99, total cost).

Concerning the planning decisions behind each solution (see Table 9), it is found that in solution A (i.e., minimum cost solution) the electricity is mainly generated from fuel 2, in solution B (an intermediate solution) electricity is generated

Table 10. Delta Values for Example 2 for All Combinations of Two Objectives^a

redu	ced set	
		delta
1	2	4.2030
1	3	21.2638
1	4	21.2638
1	5	21.2638
1	6	3.5650
1	7	21.2638
1	8	21.2638
1	9	17.7041
1	10	21.2638
1	11	21.2638
1	12	21.2638
1	13	21.2638

"Here 1 is total cost, and other objectives are environmental impacts: 2 is overall ECO₉₉, 3 is carcinogenic, 4 is respiratory organic, 5 is respiratory inorganic, 6 is climate change, 7 is ionizing radiation, 8 is layer depletion, 9 is ecotoxicity, 10 is acidification, 11 is land use, 12 is extraction of minerals, and 13 is fossil fuels.

from fuels 2 and 4, while solution C (minimum Eco-indicator 99 point) employs fuel 1.

The MILP-based dimensionality reduction method is applied next to uncover the inherent relationships among different objectives. Figure 12 shows the minimum delta value for different sets of objectives kept. As observed, the delta error diminishes with the number of objectives retained. Compared to example 1 (Figure 9), it is found that two objectives are not enough for keeping the problem structure, since no combination of two criteria manages to keep all the Pareto solutions in the reduced domain.

Table 10 displays the delta value corresponding to every possible combination of cost vs each single environmental impact, while Table 11 shows the same information, but this time for sets of three objectives. The best combination of two objectives is cost and climate change (1, 6). For three objectives, the best combination of criteria is cost, respiratory effects (inorganic), and climate change (1, 5, 6), which yields a delta error close to zero. In contrast, the pair (cost, Ecoindicator 99) leads to large delta values (i.e., 4.2). These results suggest that the use of the Eco-indicator 99 as a unique

Table 11. Delta Values for Example 2 for All Combinations of Three Objectives^a

reduced set		1	educed s	et			
			delta				delta
1	2	3	4.2030	1	5	9	17.7041
1	2	4	4.2030	1	5	10	21.2638
1	2	5	4.2030	1	5	11	21.2638
1	2	6	3.5650	1	5	12	21.2638
1	2	7	4.2030	1	5	13	21.2638
1	2	8	4.2030	1	6	7	0.8065
1	2	9	4.2030	1	6	8	0.6852
1	2	10	4.2030	1	6	9	1.3056
1	2	11	4.2030	1	6	10	0.1869
1	2	12	4.2030	1	6	11	1.4190
1	2	13	4.2030	1	6	12	1.4190
1	3	4	21.2638	1	6	13	0.2524
1	3	5	21.2638	1	7	8	21.2638
1	3	6	0.2167	1	7	9	17.7041
1	3	7	21.2638	1	7	10	21.2638
1	3	8	21.2638	1	7	11	21.2638
1	3	9	17.7041	1	7	12	21.2638
1	3	10	21.2638	1	7	13	21.2638
1	3	11	21.2638	1	8	9	17.7041
1	3	12	21.2638	1	8	10	21.2638
1	3	13	21.2638	1	8	11	21.2638
1	4	5	21.2638	1	8	12	21.2638
1	4	6	0.8065	1	8	13	21.2638
1	4	7	21.2638	1	9	10	17.7041
1	4	8	21.2638	1	9	11	17.7041
1	4	9	17.7041	1	9	12	17.7041
1	4	10	21.2638	1	9	13	17.7041
1	4	11	21.2638	1	10	11	21.2638
1	4	12	21.2638	1	10	12	21.2638
1	4	13	21.2638	1	10	13	21.2638
1	5	6	0.1869	1	11	12	21.2638
1	5	7	21.2638	1	11	13	21.2638
1	5	8	21.2638	1	12	13	21.2638
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"Here 1 is total cost, and other objectives are environmental impacts: 2 is overall ECO₉₉, 3 is carcinogenic, 4 is respiratory organic, 5 is respiratory inorganic, 6 is climate change, 7 is ionizing radiation, 8 is layer depletion, 9 is ecotoxicity, 10 is acidification, 11 is land use, 12 is extraction of minerals, and 13 is fossil fuels.

environmental metric is inadequate, since it might leave out of the analysis some Pareto solutions that perform significantly well in certain single impact categories.

6. CONCLUSION

This work proposed an approach to optimize utility plants considering the cost and several environmental indicators simultaneously. The environmental impact associated with the energy system was assessed through the Eco-indicator 99, which is based on LCA principles. The overall problem was formulated as a multiobjective MILP featuring a large number of objectives.

To overcome the numerical difficulties associated with the calculation and analysis of the Pareto solutions, we investigated the use of a rigorous dimensionality reduction method. Numerical examples show that the number of environmental objectives can be greatly reduced while still preserving the problem structure to a large extent. We observed also that the single optimization of aggregated metrics, such as the widely

used Eco-indicator 99, might change the dominance structure of the problem, leading to the potential pitfall of losing some solutions that are optimal in the original space of LCA impacts but suboptimal in the reduced domain. Our overall approach is intended to facilitate the identification of more sustainable manufacturing patterns in industry by uncovering interesting relationships between environmental and economic indicators of concern for decision-makers.

APPENDIX: MILP MODEL

Fuel Tank Models (See Section 3.1)

$$\sum_{m} TFC_{jtm}^{D} = TFC_{jt} \qquad \forall \ t, j \in TANKS$$
(18)

$$\sum_{m} \mathrm{TIC}_{jtm}^{\mathrm{D}} = \mathrm{TIC}_{jt} \qquad \forall \ t, j \in \mathrm{TANKS}$$
(19)

$$TFC_{jtm}^{D} = cost_{mt}^{FU} x_{jltm}^{FU} \theta \qquad \forall t, m, j \in TANKS, l = IN$$
(20)

$$TIC_{jtm}^{D} = cost_{mt}^{INV} \left(\frac{INVini_{jm} + INV_{jtm}}{2} \right)$$

$$\forall m, j \in \text{TANKS}, t = 1 \tag{21}$$

$$TIC_{jtm}^{D} = cost_{mt}^{INV} \left(\frac{INVini_{jt-1m} + INV_{jtm}}{2} \right)$$

$$\forall m, j \in \text{TANKS}, t > 1 \tag{22}$$

$$INV_{itm} = INVini_{im} + \theta(x_{iltm}^{FU} - x_{il'tm}^{FU})$$

$$\forall m, j \in \text{TANKS}, t = 1, l = \text{IN}, l' = \text{OUT}$$
 (23)

$$INV_{itm} = INV_{it-1m} + \theta(x_{iltm}^{FU} - x_{il'tm}^{FU})$$

$$\forall m, j \in \text{TANKS}, t > 1, l = \text{IN}, l' = \text{OUT}$$
 (24)

$$x_{it}^{\text{FU}} \text{YD}_{itm} \le x_{iltm}^{\text{FU}} \le \overline{x_{it}^{\text{FU}}} \text{YD}_{itm}$$

$$\forall t, m, j \in TANKS, l = IN, OUT$$
 (25)

$$\mathrm{INV}_{jt}\mathrm{YD}_{jtm} \leq \mathrm{INV}_{jtm} \leq \overline{\mathrm{INV}_{jt}}\mathrm{YD}_{jtm}$$

$$\forall t, m, j \in TANKS$$
 (26)

$$\sum_{m} YD_{jtm} = 1 \qquad \forall t, j \in TANKS$$
(27)

Boiler Models (See Section 3.2)

$$\sum_{m} x_{jltm}^{\text{HPD}} = x_{jlt}^{\text{HP}} \qquad \forall \ t, j \in \text{BOILERS}, \ l = \text{GEN}$$
(28)

$$x_{jltm}^{\text{HPD}} = \frac{\text{hc}_m}{\eta_{im}} x_{jl'tm}^{\text{FU}} \quad \forall t, m, j \in \text{BOILERS}, l = \text{GEN}, l'$$

$$= CON \tag{29}$$

$$\underline{x_{jt}^{\mathrm{HP}}} \mathrm{YD}_{jtm} \leq x_{jltm}^{\mathrm{HPD}} \leq \overline{x_{jt}^{\mathrm{HP}}} \mathrm{YD}_{jtm}$$

$$\forall t, m, j \in BOILERS, l = GEN$$
 (30)

$$x_{it}^{\text{FU}} \text{YD}_{itm} \le x_{iltm}^{\text{FU}} \le \overline{x_{it}^{\text{FU}}} \text{YD}_{itm}$$

$$\forall t, m, j \in BOILERS, l = CON$$
 (31)

$$\sum_{m} YD_{jtm} = 1 \qquad \forall t, j \in BOILERS$$
(32)

$$x_{jlt}^{\text{MP}} = a_j^{\text{MP}} x_{jl't}^{\text{HP}} \quad \forall t, j \in \text{BOILERS}, l = \text{CON}, l'$$

$$= \text{GEN}$$
(33)

$$x_{jlt}^{\text{EL}} = a_j^{\text{EL}} x_{jl't}^{\text{HP}} \quad \forall t, j \in \text{BOILERS}, l = \text{CON}, l'$$

$$= \text{GEN}$$
(34)

$$\sum_{j \in \text{BOILERS}} x_{j|lm}^{\text{FU}} = \sum_{j \in \text{TANKS}} x_{j|'tm}^{\text{FU}}$$

$$\forall t, m, l = CON, l' = OUT$$
 (35)

Turbine Models (See Section 3.3)

$$x_{jlt}^{\text{EL}} = b_j^{\text{HP}} x_{jl't}^{\text{HP}} - g_j^{\text{MP}} x_{jlt}^{\text{MP}} - g_j^{\text{LP}} x_{jlt}^{\text{LP}} - g_j^{\text{CO}} x_{jlt}^{\text{CO}}$$

$$\forall t, j \in \text{TURBINES}, l = \text{GEN}, l' = \text{IN}$$
(36)

$$\underline{x_{jlt}^{\text{EL}}} \leq x_{jlt}^{\text{EL}} \leq \overline{x_{jlt}^{\text{EL}}} \qquad \forall \ t, j \in \text{TURBINES}, \ l = \text{GEN}$$
 (37)

$$x_{jlt}^{HP} = x_{jl't}^{MP} + x_{jl't}^{LP} + x_{jl't}^{CO}$$

$$\forall t, j \in \text{TURBINES}, l = \text{IN}, l' = \text{GEN}$$
(38)

Demand Satisfaction (See Section 3.4)

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{EL}} + \text{EPU}_t - \sum_{j \in \text{BOILERS}} \sum_{l = \text{CON}} \theta x_{jlt}^{\text{EL}}$$

$$\geq \operatorname{dem}_{t}^{\operatorname{EL}} \quad \forall \ t$$
 (39)

$$\sum_{j \in \text{BOILERS}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{HP}} - \sum_{j \in \text{TURBINES}} \sum_{l = \text{IN}} \theta x_{jlt}^{\text{HP}} \ge \text{dem}_t^{\text{HP}}$$

$$\forall t$$
 (40)

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{MP}} - \sum_{j \in \text{BOILERS}} \sum_{l = \text{CON}} \theta x_{jlt}^{\text{MP}} \ge \text{dem}_t^{\text{MP}}$$

$$\forall t$$
 (41)

$$\sum_{j \in \text{TURBINES}} \sum_{l = \text{GEN}} \theta x_{jlt}^{\text{LP}} \ge \text{dem}_t^{\text{LP}} \qquad \forall \ t$$
(42)

Objective Functions

Total Cost (See Section 3.5.1).

$$\begin{aligned} \text{TC} &= \sum_{j \in \text{TANKS}} \sum_{t} \text{TFC}_{jt} + \sum_{j \in \text{TANKS}} \sum_{t} \text{TIC}_{jt} \\ &+ \sum_{t} \text{cost}_{t}^{\text{EL}} \text{EPU}_{t} \end{aligned} \tag{43}$$

Environmental Impacts (See Section 3.5.2).

$$\begin{split} \text{LCI}_b &= \text{LCI}_b^{\text{FU}} + \text{LCI}_b^{\text{EL}} + \text{LCI}_b^{\text{DE}} \\ &= \sum_{i \in \text{TANKS}} \sum_{l = \text{IN}} \sum_{t} \sum_{m} \theta \omega_{mb}^{\text{FU}} x_{jltm}^{\text{FU}} + \sum_{t} \omega_b^{\text{EL}} \text{EPU}_t \end{split}$$

+
$$\sum_{j \in \text{BOILERS}} \sum_{l=\text{CON}} \sum_{t} \sum_{m} \theta \omega_{mb}^{\text{DE}} x_{jltm}^{\text{FU}} \qquad \forall b$$
 (44)

$$IM_c = \sum_b df_{bc} LCI_b \qquad \forall c$$
(45)

$$DAM_{d} = \sum_{c \in ID_{d}} IM_{c} \qquad \forall d$$
(46)

$$ECO_{99} = \sum_{d} n_d w_d DAM_d \tag{47}$$

Notation

Indices

b =chemical species

c = impact categories

d =damage categories

i = process units

l = material state

m = fuels

t =time periods

Sets

BOILERS = set of process units j which are boilers ID = set of impacts c contributing to damage category dTANKS = set of process units j which are tanks

TURBINES = set of process units j which are turbines

 a_i^{MP} = material balance coefficient for medium pressure steam in unit j, ton/ton

cost^{ELI}_t = cost of electricity in period t, \$/(MW·h) cost^{FU}_{mt} = cost of fuel m in period t, \$/ton cost^{INV}_{mt} = unitary inventory cost associated with fuel m and period t, $\frac{s}{(ton \cdot h)}$

 DEM_t^{EL} = demand of electricity in period t, MW/h

DEM_t^{HP} = demand of Electricity in period t, tww/in DEM_t^{LP} = demand of HP steam in period t, ton/h DEM_t^{LP} = demand of LP steam in period t, ton/h

 DEM_t^{MP} = demand of MP steam in period t, ton/h

 df_{bc} = damage factor associated with chemical b and impact c, impact/(kg (MJ))

 g_i^{CO} = material balance coefficient for condensate in unit j, MW·h/ton

 g_i^{LP} = material balance coefficient for low pressure steam in unit j, MW·h/ton

 g_i^{MP} = material balance coefficient for medium pressure steam in unit j, MW·h/ton

 $hc_m = heat of combustion of fuel m, kJ/ton$

 n_d = normalization factor associated with damage category d w_d = weighting factor associated with damage category d

 INV_{it} = lower bound on the inventory of fuel in unit j in period t, ton

 $\overline{INV_{it}}$ = upper bound on the inventory of fuel in unit j in

 $INVini_{itm} = initial inventory of fuel$ *m*in unit*j*, ton

 x_{ilt}^{EL} = lower bound on flow of electricity in state l in unit j in

 $\overline{x_{ilt}^{\text{EL}}}$ = upper bound on flow of electricity in state l in unit j in period t, MW

 x_{it}^{FU} = lower bound on flow of fuel in unit *j* in period *t*, ton/h

 $\overline{x_{it}^{\text{FU}}}$ = upper bound on flow of fuel in unit j in period t, ton/h x_{ilt}^{EL} = lower bound on flow of electricity in state *l* in unit *j* in period t, MW

 $\overline{x_{ilt}^{\text{EL}}}$ = upper bound on flow of electricity in state *l* in unit *j* in period t, MW

 x_{it}^{HP} = lower bound on flow of high pressure steam in unit j in period *t*, ton/h

 $\overline{x_{it}^{\text{HP}}}$ = upper bound on flow of high pressure steam in unit j in period t, ton/h

 ϵ = auxiliary parameter employed in epsilon constraint method

 θ = length of a time period, h

 η_{im} = efficiency of boiler *j* combusting fuel *m*, kJ/ton

 $\omega_{mb}^{\rm DE}$ = life cycle inventory entry associated with chemical b per unit of fuel *m* combusted

 $\omega_b^{\rm EL}$ = life cycle inventory entry associated with chemical b per unit of external electricity purchased

 $\omega_{mb}^{\rm FU}$ = life cycle inventory entry associated with chemical b and fuel m per unit of fuel m generated

Variables

 DAM_d = impact in damage category d, impact/(kg (MJ))

 ECO_{99} = Eco-indicator 99 value, ecopoints

 EPU_t = purchases of external electricity in period t, MW $IM_c = damage in impact category c, DALYs, PDF·m²·year,$

 INV_{itm} = inventory of fuel m in unit j in period t, ton

 LCI_b = life cycle inventory associated with chemical b

 LCI_{b}^{DE} = life cycle inventory associated with chemical b due to direct emissions

 LCI_b^{EL} = life cycle inventory associated with chemical b due to consumption of external electricity

 LCI_b^{FU} = life cycle inventory associated with chemical b due to generation of fuel

 TIC_{jt}^{D} = total cost of inventory in unit j in period t, \$ TIC_{jtm}^{D} = total cost of inventory of fuel m in unit j in period t(disaggregated variable for convex hull reformulation), \$

TFC_{jt} = total cost of fuel in unit j in period t, \$
TFC^D_{jtm} = total cost of fuel m in unit j in period t (disaggregated variable for convex hull reformulation), \$ TC = total cost, \$

 x_{ilt}^{CO} = flow rate of condensate in state *l* in unit *j* in period *t*, ton/h

 x_{ilt}^{EL} = flow rate of electricity in state *l* in unit *j* in period *t*, МW

 $\alpha_{jltm}^{\rm FU}$ = flow rate of fuel m in state l in unit j in period t, ton/h $\alpha_{jlt}^{\rm HP}$ = flow rate of high pressure steam in state l in unit j in period *t*, ton/h

 x_{iltm}^{HPD} = flow of high pressure steam in unit j in period t in mode l when fuel m is used in that unit (disaggregated variable for convex hull reformulation), ton/h

 x_{ilt}^{LP} = flow rate of low pressure steam in state *l* in unit *j* in period t, ton/h

 x_{ilt}^{MP} = flow rate of medium pressure steam in state *l* in unit *j* in period *t*, ton/h

 YD_{itm} = binary variable (1 if fuel m is selected in unit j in period *t*, 0 otherwise)

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Notes

The authors declare no competing financial interest.

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