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Ecodesign of Chemical Processes with Multi-Objective Genetic Algorithms

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12.1 Introduction

Since the early 2000s, due to increasingly stringent environmental concerns, environmental objectives have been considered together with classical technical and/or economic criteria, in most engineering fields, particularly in chemical engineering [1]. So traditional single objective process optimization has been progressively transformed into multi-objective optimization, where the problem consists of optimizing a vector $[f_1, f_2, \ldots, f_k]^{\mathrm{T}}$ of objectives under a set of constraints. As far as the set R^k is not provided with an order relation, classical techniques of single objective optimization field, like gradient methods, cannot be implemented to solve a multi-objective optimization (MOO) problem.

According to [2], multi-objective optimization procedures can be broadly classified into two categories –scalarization methods on the one hand, and genetic and evolutionary methods on the other hand. Scalarization methods apply in mathematically well defined problems with explicit formulations of objectives and constraints, whereas genetic and evolutionary methods based on evolutionary strategies mainly apply in black-box problems, where objectives and/or constraints are evaluated by a computer code for each value of the optimization variable set. Besides black-box problems, the possibility to mutate out of a local optimum and the ability to compute the entire Pareto front in one run make this type of method attractive. In the former group of methods, the multi-objective optimization problem is transformed into a single (or a series of) single objective problem(s). An interesting review of various techniques is given in [3]. Seven types of scalarization methods are presented

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in [4], but the two most popular ones are undoubtedly the weighted sum (WS) [5] and the ε-constraint (ε-C) [6] procedures.

In the latter class of genetic and evolutionary methods, each objective function is considered separately during the optimization phase; these approaches typically implement the notion of dominance to distinguish between dominated and non-dominated solutions.

Both classes of methods have their own drawbacks: scalarization methods need to check mathematical properties such as convexity, which may be very difficult to implement for complex engineering problems; for problems involving crisp equality constraints (like balance equations for example), an external solver has to be used for each point generated by a genetic and evolutionary method.

Moreover, the efficiency of a given method for a particular example is hardly predictable, and according to the *no free lunch (NFL) theory* [7], there is no method that surpasses all the other ones for any considered problem. Insofar as industrial packages (ARIANE^{TM}) [8] are used for computing environmental objectives in the second example of this chapter, the problem is a black-box one, and an evolutionary strategy has been adopted to solve it.

After the complete set of solutions of the MOO problem (i.e. the Pareto front) is found, the next step consists in identifying the best ones. There are a variety of multiple choice decision–making (MCDM) procedures to aid the decision maker in a multiple criteria situation. In chemical engineering field, one of the most popular MCDM methods is TOPSIS for identifying solutions from a finite set of alternatives based upon simultaneous minimization of distance from an ideal point and maximization of distance from the nadir point. The acronym TOPSIS stands for technique for order preference by similarity to the ideal solution. The first TOPSIS developments were carried out by Hwang and Yoon (1981) [9] and later by Lai *et al.* (1994) [10]. Among the MCDM methods, TOPSIS is attractive because it requires limited subjective inputs from decision makers. The only subjective inputs needed are weights assigned to objectives. This may explain why TOPSIS [11] is very popular in chemical engineering applications; it has been adopted in this study together with a simple code based on Pareto ranking, called FUCA, as an alternative MCDM technique.

The numerical tools and methods used in this chapter will be briefly presented in section 12.2. Then, two typical chemical engineering problems will illustrate the concepts. The first chemical engineering MOO problem tackled in section 12.3 is related to the Williams and Otto process (WOP). This small-sized fictitious plant first proposed in [12] is realistic and involves many of the features of a real process. It has served as a benchmark for many researchers (for instance, [13] [14] [15]). An interesting contribution to the case of multi-objective optimization is proposed in [16] in which the problem is analysed from an economic viewpoint with profitability criteria as objective functions. In this chapter, economic objectives are optimized together with an environmental criterion, namely the flow rate of the heavy oil F_G considered as a waste. Two tri-objective MOO problems are solved, i.e., [Max *NPW*, Max *PBT*, Min F_G] and [Max *NPW*, Min *PBP*, Min F_G], where *NPW* is the net present worth value, *PBT*, the profit before taxes and *PBP*, the payback period respectively. An analysis of the influence of the third environmental criterion on the two first economic objectives is carried out.

In section 12.4, the second illustration example is devoted to the presentation of the HDA process revisited here in a multi-objective way with some of the criteria involved in sustainable assessment. It must be emphasized that optimization for sustainability is a

complex and challenging task, both due to the number of criteria that may be involved and also to the subjective criteria that may be difficult to formulate mathematically. This chapter only considers two pillars of sustainable development: the economic and environmental components.

12.2 Numerical Tools

12.2.1 Evolutionary Approach: Multi-Objective Genetic Algorithms

The two most popular evolutionary methods in the chemical engineering field are MGA (multi-objective genetic algorithm [17]), and MOSA (multi-objective simulated annealing, [18]). Neither method is perfect and selecting one depends on the requirements of the particular design situation considered. From [19], [20] and [21], it appears that MGA is generally preferred to MOSA. One of the most efficient genetic algorithms is NSGA II [22], an upgrade of NSGA, which estimates the density of solutions surrounding a particular one, in order to perform an efficient scanning of the solution space. Its performance is so good that it has gained a lot of popularity in recent years [23].

The MOO procedure implemented in this chapter is the NSGA II-modified SBX described in [24]. This crossover operator differs from that in the first NSGA II version by the crossover probability allocation for each gene. Compared with the classical NSGA II version, the global probability of crossover per gene is higher in the modified SBX. Consequently, this new crossover operator performs more efficient gene mixing [24].

Furthermore, when clones are generated by the crossover operation, the modified SBX implements a forced mutation of children. The goal is to avoid unnecessary calculations of clones. All the children generated by the reproduction scheme are statistically different.

12.2.2 Choice of the Best Solutions

The next step consists, then, of identifying the best ones among those of the Pareto front. This MCDM issue is also a complex problem, mainly because of its more subjective nature. Some generic tools like ELECTRE [24], PROMETHEE [25] [26] and TOPSIS [11] are commonly used in many engineering and economic fields. However, TOPSIS remains one of the most popular methods in chemical engineering applications.

The fundamental concept of the TOPSIS method is the use of Euclidian distances to choose the best alternative. TOPSIS is a synthetic evaluation method, where the distance between available solutions and the “optimized ideal reference point” is calculated. The optimized ideal reference point is a theoretical point where objectives are at their optimal values. The method calculates the distance between the ideal reference and each point of the Pareto curve, and ranks them by increasing order of distances. The procedure starts with a decision matrix that contains all the alternatives ordered by the criteria and a weight vector is defined. The following step is to calculate the normalized decision matrix, after the positive and negative ideal solutions are defined from the standardized matrix. Then, the separation measures of each alternative are calculated and, finally, a ratio for each alternative is estimated. The alternatives are ranked according to their ratio. Unless explicitly mentioned, TOPSIS has been adopted in this study.

12.3 Williams–Otto Process (WOP) Optimization for Multiple Economic and Environmental Objectives

This engineering problem was first proposed in [12] and used by many researchers as a benchmark for constrained NLP studies [27] [28] and recently in bi-objective economic optimization [16] [29]. This fictitious process [15] contains many of the characteristics of a typical chemical plant while being realistic enough. The plant is to manufacture a given amount of a chemical product P per year; it consists of a perfectly stirred reactor, a heat exchanger, a decanter and a distillation column in series (see Figure 12.1). There is a recycle stream from the column reboiler to the reactor, where three second-order irreversible reactions occur. Reactants A and B are fed separately to the reactor in pure form, together with the recycled stream, where the desired product P is produced. Component C is an intermediate product (with no sale value), component E is a byproduct and component G is a heavy oil considered as a waste material. To prevent accumulation of byproduct E, a part of the column bottom is purged (purge rate ξ), while the most of it is recycled to the reactor. As the purged stream has a substantial fuel sale value, it is sold. The production of the desired product P (F_P) is assumed to be set at 2160 kg/h.

12.3.1 Process Modelling

The reactions occurring in the reactor are:

$$A + B \xrightarrow{k_1} C$$
$$C + B \xrightarrow{k_2} P + E$$
$$P + C \xrightarrow{k_3} G$$

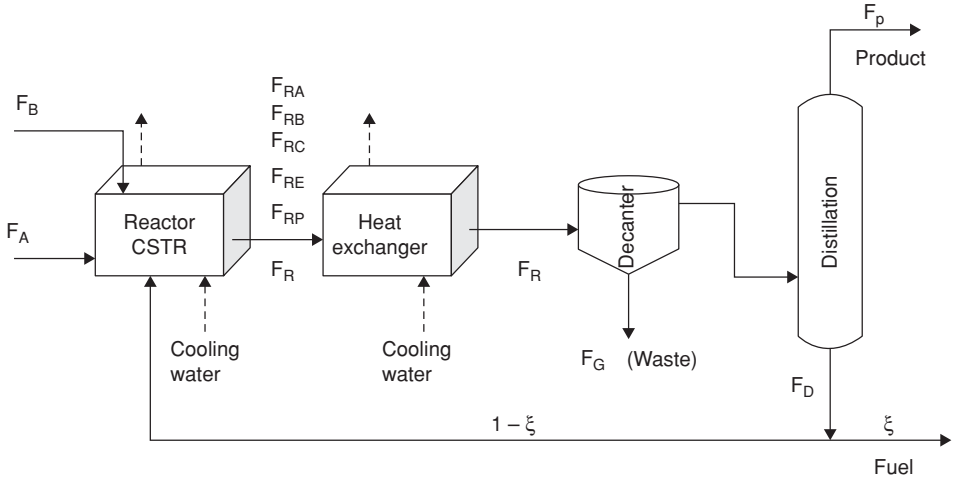

Figure 12.1 *Williams–Otto process.*

Table 12.1 *Arrhenius constants.*

	i = 1	i = 2	i = 3
A_i (h^{-1})	$5.9755\ 10^9$	$2.5962\ 10^{12}$	$9.6283\ 10^{15}$
B_i (K)	6,666.67	8,333.33	11,111.11

where constants k_1, k_2 and k_3 are determined from the Arrhenius law (see Table 12.1):

$$k_i = A_i \exp(-B_i/1.8T) \tag{12.1}$$

The modelling equations can be expressed as:

- Mass balance on component A

$$h_1 = F_A + (1-\xi)F_{RA} - (k_1 W_A W_B)\, V\rho - F_{RA} = 0 \tag{12.2}$$

- Mass balance on component B

$$h_2 = F_B + (1-\xi)F_{RB} - (k_1 W_A + k_2 W_C)\, W_B V\rho - F_{RB} = 0 \tag{12.3}$$

- Mass balance on component C

$$h_3 = (1-\xi)\ F_{RC} + (2\ k_1 W_A W_B - 2\ k_2 W_B W_C - k_3 W_P W_C)\ \ V\rho - F_{RC} = 0 \tag{12.4}$$

- Mass balance on component E

$$h_4 = (1-\xi)\ F_{RE} + (2\ k_2 W_B W_C)\ \ V\rho - F_{RE} = 0 \tag{12.5}$$

- Mass balance on component P

$$h_5 = [k_2 W_B W_C - 0,5\ k_3 W_P W_C)\ \ V\rho - 0,1\xi F_{RE} - F_P = 0 \tag{12.6}$$

- Mass balance on component G

$$h_6 = (1-\xi)\ F_{RC} + (2\ k_1 W_A W_B - 2\ k_2 W_B W_C - k_3 W_P W_C)\ \ V\rho - F_{RC} = 0 \tag{12.7}$$

- with:

$$W_i = \frac{F_{Ri}}{\sum\limits_i F_{Ri}} \qquad\qquad i = \text{A, B, C, E, P, G} \tag{12.8}$$

12.3.2 Optimization Variables

The mathematical model involves 10 variables, F_A, F_B, F_G, F_{RA}, F_{RB}, F_{RC}, F_{RE}, η, V et T, and six nonlinear equations (12.2 to 12.7), that is to say four degrees of freedom. Based on the work proposed in [16], the chosen decision variables are the mass flow rate of reactant B (F_B), the reactor volume (V), the reactor temperature (T), and the purge rate (ξ).

12.3.3 Objectives for Optimization

12.3.3.1 Economic Objectives ([15], [16])

Fixed capital cost *FCI* is the capital necessary for the installed process equipment with all components needed for complete operation process:

$$FCI = \frac{600\,V\rho}{0.453}(\$) \tag{12.9}$$

where V is the reactor volume (m^3) and ρ the density of the material. Operating cost C_{op} is the cost corresponding to the plant in operation, excluding the depreciation cost:

$$C_{op} = \frac{1}{0.453}(168F_A + 252F_B + 2.22(F_{recycle} + F_A + F_B) + 84F_G) + 1,041.6\ (\$) \tag{12.10}$$

The total annual cost *TAC* is the sum of operating cost C_{op} and the depreciation cost. This depreciation cost is computed by the so-called straight-line method by dividing the fixed capital cost *FCI* over the lifetime of the project (assumed to be 10 years):

$$TAC = C_{op} + \frac{FCI}{10}(\$) \tag{12.11}$$

The profit before taxes *PBT* is the difference between the annual revenue and *TAC*, without accounting for taxes. The annual revenue is made up of the sale prices of product *P* and the purged column bottom:

$$PBT = \frac{1}{0.453}(2,207F_P + 50F_{purge}) - TAC \quad (\$/\text{an}) \tag{12.12}$$

The annual cash flow *CF* is the sum of profit after taxes and depreciation, where the tax rate r_t is fixed at 30% per year. Depreciation and *CF* are assumed to be the same every year during the project life.

$$\begin{aligned} CF = (1 - r_t)\Bigg[&\frac{1}{0.453}((0.453PBT + TAC) - 168F_A - 252F_B) \\ &-2.22(F_{recycle} + F_A + F_B) - 84F_G) - 1,041.6\Bigg] + 0.3r_t\left[\frac{60V\rho}{0.453}\right]^{(\$/\text{an})} \end{aligned} \tag{12.13}$$

The payback period *PBP*, to be minimized, is the length of time necessary to pay out the capital investment by using the annual net cash flow that returns to the company's capital reservoir *FCI*.

$$PBP = \frac{FCI}{CF}(\text{year}) \tag{12.14}$$

The net present worth value *NPW*, to be maximized, is the present value of all investments and cash flows during the project lifetime. *NPW* considers the time value of the earned money. In the expression of *NPW*, *TCI* is the total capital investment and $f_{PA}(i)$ is the present worth annuity factor, the expected rate of return i (also called discount rate) is taken

as 0.12 year^{-1}. The net present value takes into account all expected annual earnings—the annual net cash flows—and discounts them to today's value.

$$NPW = -TCI + f_{PA}(i)CF \quad (\$) \tag{12.15}$$

$$f_{PA}(i) = \frac{(1+i)^{10} - 1}{i(1+i)^{10}} (\text{year}) \tag{12.16}$$

For performing the WOP optimization, a constant *CF* and no working capital are assumed (in that case, $TCI = FCI$).

Among the three economic objectives *NPW*, *PBT* and *PBP*, *NPW* is the more important one because it considers the cash flows over the project lifetime and the time value of the money; so solutions with a larger *NPW* would be better.

12.3.3.2 Environmental Objective

The consideration of the environmental aspects of the process and the plant plays an ever increasing role. So other objectives linked to the environmental impact must be simultaneously considered together with the economic objectives. In the WOP, we assume that all the pollutants generated by the process are concentrated in the heavy oil obtained at the decanter bottom. So the WOP MOO problem consists of optimizing economic objectives together with the environmental criterion, that is to say, the flow rate F_g, to be minimized.

12.3.4 Problem Constraints

According to [16], the four independent variables are bounded as follows:

$$10\,000 \leq F_B \leq 15\,000 \text{ kg/h}$$
$$0.85 \leq V \leq 10 \text{ m}^3$$
$$322 \leq T \leq 378 \text{ K}$$
$$0 \leq \eta \leq 0.99$$

The six nonlinear constraints correspond to the set of equations (12.2–12.7).

12.3.5 Implementation

The MOO problem is implemented under the MS Excel environment interfaced with the Matlab toolbox for solving the set of the six nonlinear constraints (Equations 12.2 to 12.7), as displayed in Figure 12.2. The initial values used for solving the nonlinear system are obtained from [27] (see Table 12.2). The parameters of the genetic algorithm are indicated in Table 12.3.

12.3.6 Procedure Validation

The procedure was validated by performing, as a first step, economic bi-objective optimizations, and the results were compared with those of [16]. For the problem [Max *NPW*, Max *PBT*] (respectively [Max *NPW*, Min *PBP*]) the Pareto front is displayed in Figure 12.3 (respectively Figure 12.4), where the point A1 (respectively B1) is the best solution according to the TOPSIS ranking. The corresponding variable and objective values are listed in

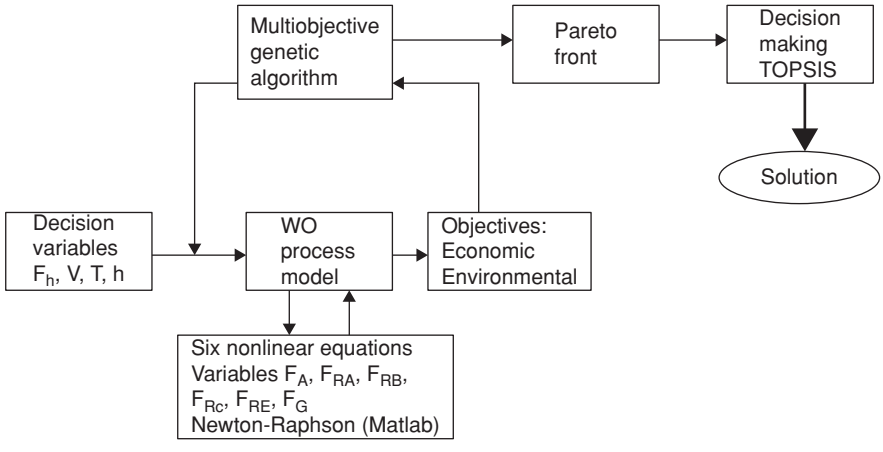

Figure 12.2 *Strategy for optimizing the WOP.*

Table 12.4, where those obtained in [16] are also reported. The relative difference d between two values a and b (a value obtained in this study, b value reported in [16]) is computed as:

$$d = 100 \times \frac{|a - b|}{0.5 \times (a + b)} \tag{12.17}$$

For the problem [Max *NPW*, Max *PBT*] (respectively [Max *NPW*, Min *PBP*]) the mean relative difference between both investigations is 1.51% (respectively 5.47%). This is mainly due to the difference in reactor volume. From a numerical point of view, the genetic algorithms used in the two studies are different (NSGA II aJG [16] and NSGA II-modified

Table 12.2 *Initial values used for solving the nonlinear equations.*

Initial values		
F_A	(kg/h)	6136
F_{RA}	(kg/h)	8239
F_{RB}	(kg/h)	27 594
F_{RC}	(kg/h)	1509
F_{RE}	(kg/h)	27 426
F_G	(kg/h)	1635

Table 12.3 *Parameters of the genetic algorithm.*

Population size	200
Number of generations	1000
Crossover probability	0.75
Mutation probability	0.20

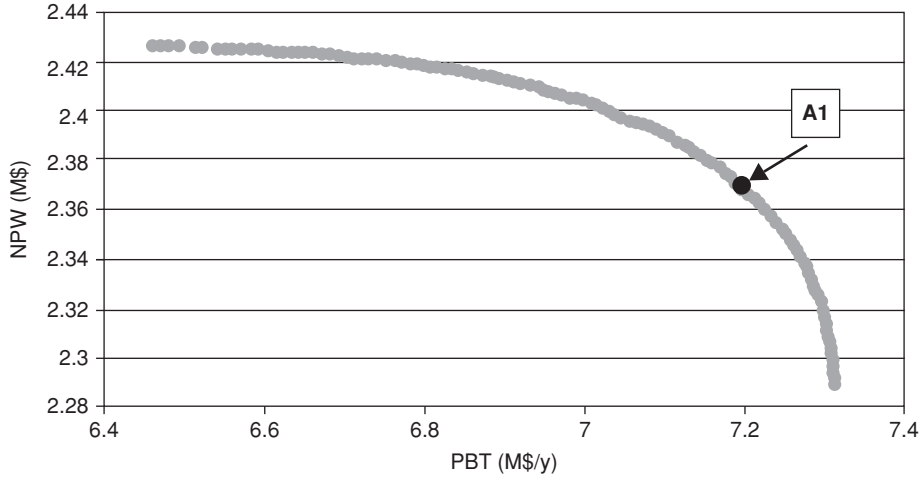

Figure 12.3 *Pareto front for the problem [Max* NPW*, Max* PBT*].*

SBX in this work), so the solutions generated are slightly different. Yet, the differences remain very acceptable.

In this study, the flow rate F_G of pollutant G is 1,135.18 kg/h, while in [16], this value is 1,211.36 kg/h. The aim of the tri-objective optimization of the WOP presented in the following section is to reduce this pollutant flow rate, while maintaining a good economic efficiency for the process.

12.3.7 Tri-Objective Optimization

This study was carried out in a PhD thesis by A. Ouattara (2011) [30]. The economic objectives are now optimized together with the environmental criterion, namely the flow rate of heavy oil F_G.

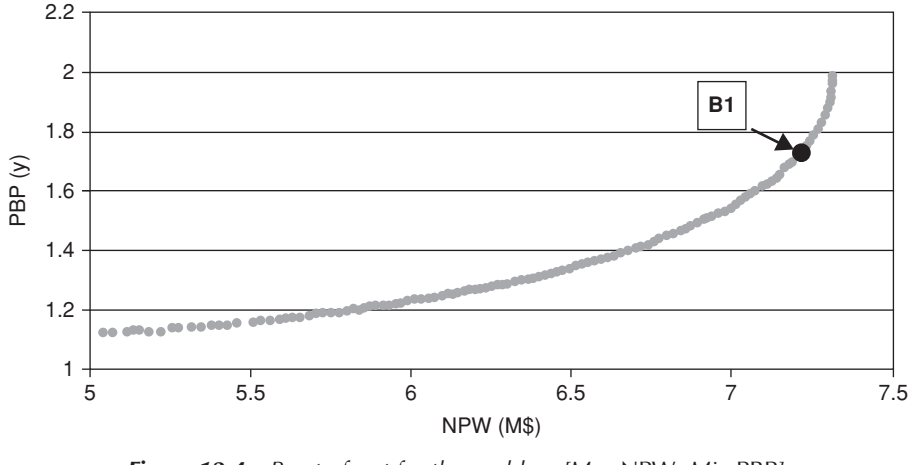

Figure 12.4 *Pareto front for the problem [Max* NPW*, Min* PBP*].*

Table 12.4 *Values obtained from bi-objective optimizations.*

	[Max *NPW*, Max *PBT*]			[Max *NPW*, Min *PBP*]		
Variable	This study	Lee *et al.* [16]	Diff.%	This study	Lee *et al.* [16]	Diff.%
F_B, kg/h)	11,519.87	11,600	0.69	12,090.32	12,100	0.08
V (m^3)	4.70	4.41	6.37	2.28	3.09	30.17
T (K)	347.86	348.90	0.30	354.78	354.70	0.02
η	0.11	0.11	0	0.11	0.11	0
NPW (M$)	7.20	7.26	0.83	7.21	7.23	0.28
PBT (M$)	2.37	2.35	0.85	1.72	1.76	2.30

12.3.7.1 Case 1: [Max NPW*, Max* PBT*, Min* F_G*]*

As can be observed on the three-dimensional Pareto front displayed in Figure 12.5, when *NPW* and *PBT* increase, F_G increases too. When the economic efficiency of the WOP increases, its environmental impact becomes worse. As it is well known in industrial practice, economic and environmental objectives are most of the time antagonistic. In order to determine a good tradeoff between economic and environmental point of view, a TOPSIS ranking was carried out on the set of points of the Pareto front. Assuming the same weight for the three objectives, the best solution identified by TOPSIS is C1 as displayed in Figure 12.5.

The differences between the results obtained in the bi and tri-objective optimizations are reported in Table 12.5. For variables F_B, V, T, η and objectives *NPW* and *PBT*, the mean difference is 8.41%. As expected, the reactor volume becomes higher, leading to a decrease

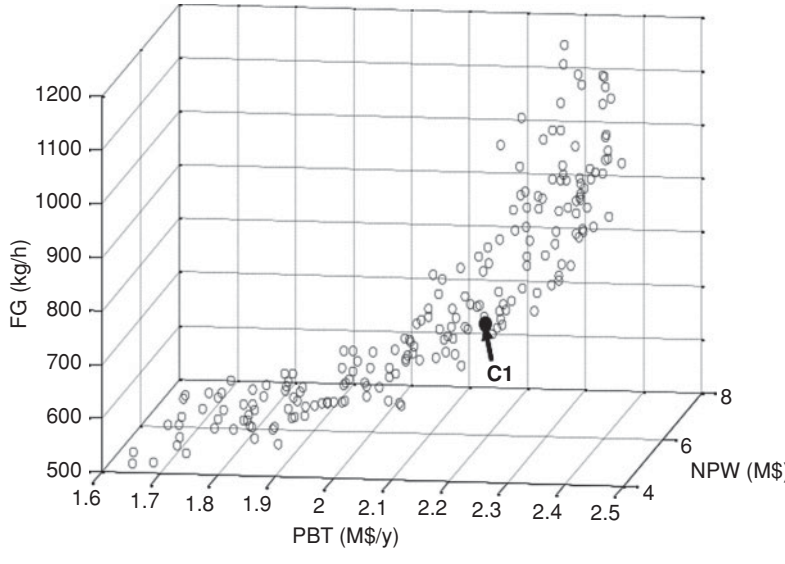

Figure 12.5 *Pareto front for the problem [Max* NPW*, Max* PBT*, Min* F_G*].*

Table 12.5 *Differences between bi and tri-objective optimizations for the problem [Max* NPW*, Max* PBT*, Min* F_G*].*

Variable	Bi-objective	Tri-objective	Diff.%
F_B (kg/h)	11 519.87	11 728.10	1.79
V (m^3)	4.70	5.56	16.76
T (K)	347.86	340.37	2.18
η	0.11	0.10	9.52
NPW (M$)	7.20	6.25	14.13
PBT (M$)	2.37	2.23	6.09
F_G (kg/h)	1135.18	750.89	40.7

in the economic objectives *NPW* and *PBT*, while the flow rate F_G of pollutant strongly decreases (40.7%).

12.3.7.2 Case 2: [Max NPW*, Min* PBP*, Min* F_G*]*

From the three-dimensional Pareto fronts shown in Figure 12.6, when F_G decreases, *PBP* increases. When *PBP* decreases, *NPW* becomes higher, and F_G and *NPW* increase together. This behaviour shows, as in the first case, the antagonistic nature of economic and environmental objectives. Assuming always the same weight for the three objectives, a TOPSIS ranking was carried out and the best solution identified by TOPSIS is C2 in Figure 12.6.

Table 12.6 shows the differences between the results obtained in the bi- and tri-objective optimizations. For the variables F_B, V, T, η and objectives *NPW* and *PBP*, the mean difference is 11.73%.

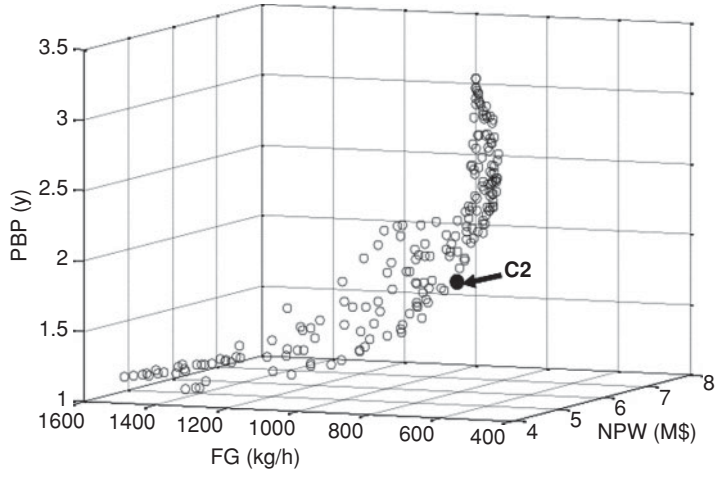

Figure 12.6 *Pareto front for the problem [Max* NPW*, Min* PBP*, Min* F_G*].*

Table 12.6 *Differences between bi and tri-objective optimizations for the problem [Max* NPW*, Min* PBP*, Min* F_G*].*

Variable	Bi-objective	Tri-objective	Diff.%
F_B (kg/h)	12 090.32	12 725.31	5.12
V (m^3)	2.28	2.68	16.13
T (K)	354.78	351.63	0.89
η	0.11	0.10	9.52
NPW (M$)	7.21	6.32	13.16
PBT (M$)	1.72	1.75	1.73
F_G (kg/h)	1211.36	845.62	35.56

12.3.8 Discussion

The tri-objective optimization highlights the well-known antagonism between economic and environmental concerns. Compared to bi-objective economic optimization, in the former case related to [Max *NPW*, Max *PBT*, Min F_G], the more important economic objective, which is the net present worth value *NPW*, decreases by 14% and the secondary economic criterion, the profit before taxes *PBT,* falls by 6%, while the waste rejection is decreased by 40%. In the latter case concerning [Max *NPW*, Min *PBP*, Min F_G] (where *PBP* is the payback period), these values are respectively equal to 13%, 2% and 36%. So from an environmental point of view, tri-objective optimization yields big savings, while not affecting the economic criteria too adversely.

12.4 Revisiting the HDA Process

The so-called HDA process is dedicated to the production of benzene by hydrodealkylation of toluene. This plant is a hypothetical study, based on the type of design project set by the Institution of Chemical Engineers (IChemE). Due to its hypothetical nature, some of the assumptions and design decisions may not be realistic. Moreover, the data concerning the production capacity, the market prices of raw materials, utilities and products may not correspond to the actual situation. We think that this limitation is not prejudicial, as our goal is to illustrate how multi-objective optimization strategies can be useful for taking into account sustainability criteria at the preliminary design phase. It must be also emphasized that this example is far from being the best example to demonstrate the wide spectrum of applications that can be deduced from a multi-objective optimization study: indeed the HDA processing route being well established, only few choices concerning the process, technologies and raw materials can be made at the first design stage.

12.4.1 HDA Process Description and Modelling Principles

The hydrodealkylation process [31] is a classical method for benzene production. This process involves two reactions, i.e., the conversion of toluene to benzene (Equation 12.18)

and the equilibrium between benzene and diphenyl (Equation 12.19).

$$toluene + H_2 \rightarrow benzene + CH_4 \tag{12.18}$$

$$2benzene \leftrightarrow diphenyl + H_2 \tag{12.19}$$

Based on a hierarchical design/synthesis approach, this process has been studied extensively by Douglas (1988) [31]. The purity of the hydrogen-feed stream is 95% and it involves 5% of methane. Fresh inlet stream of toluene, recycled toluene, and recycled hydrogen are mixed with this feed stream. The feed mixture is heated in a furnace before being fed to an adiabatic reactor. Unreacted hydrogen and toluene, benzene (the desired product), biphenyl, and methane constitute the reactor effluent, which is quenched and subsequently cooled in a high-pressure flash separator to separate the aromatics from the noncondensable hydrogen and methane. The vapour steam produced by the high-pressure flash unit contains hydrogen and methane that is recycled. Traces of hydrogen and methane from the liquid stream are separated from the aromatics in a low-pressure flash drum. This drum produces a stream composed of benzene, biphenyl and toluene that are separated in two distillation towers. The first column isolates the product, benzene, from biphenyl and toluene, while the second one separates the biphenyl from toluene, which is recycled at the reactor entrance. Energy is saved by using the outlet stream leaving the reactor as its temperature is 620 °C, to preheat the feed stream coming from the mixer via a heat exchanger (Fehe); in that way, some energy integration is achieved. Figure 12.7 presents the process flow diagram (PFD) for the production of benzene via HDA.

To model the HDA process, commercial design and flow-sheeting packages could be used to predict the performance of the processes in order to compute the objective functions that will be used further during the optimization step. However, rather than using such packages, the equations proposed by Douglas (1988) [31] have been directly implemented and solved by the Excel® solver. The main objective is to solve material and energy balances to obtain the flow rates and enthalpies in each stream of the process. Diphenyl has been considered as a pollutant.

When considering environmental impacts generated by a process, it is necessary to broaden the frontier of the system, thus embedding the primary energy requirement of the given process. Of course, the approach would be more environmentally sound if a life-cycle assessment (LCA) methodology is developed for analysing and assessing the environmental impact of the benzene product throughout the entire life cycle.

A complete life cycle includes all processes from the cradle to the grave—raw material, extraction, processing, transportation, manufacturing, distribution, use, reuse, maintenance, recycling and waste treatment. This holistic approach is very tedious because it is difficult to consider a LCA approach based on the only value of benzene, which is, however, an important commodity chemical used in a large range of applications. This is why the approach developed here, which is an oriented LCA approach, only focused on the impact generated by both the process and its associated utility production. Following sustainability guidelines, a set of metrics or indicators have been developed by IChemE (2003) [32], AIChE (1988) [33] and CSD (1996) [34]. Environmental burdens, defined as quantitative measures of the potential contributions of substances released to a particular environmental potential impact, are used to define these indicators. They are often limited to a cradle-to-gate or gate-to-gate study.

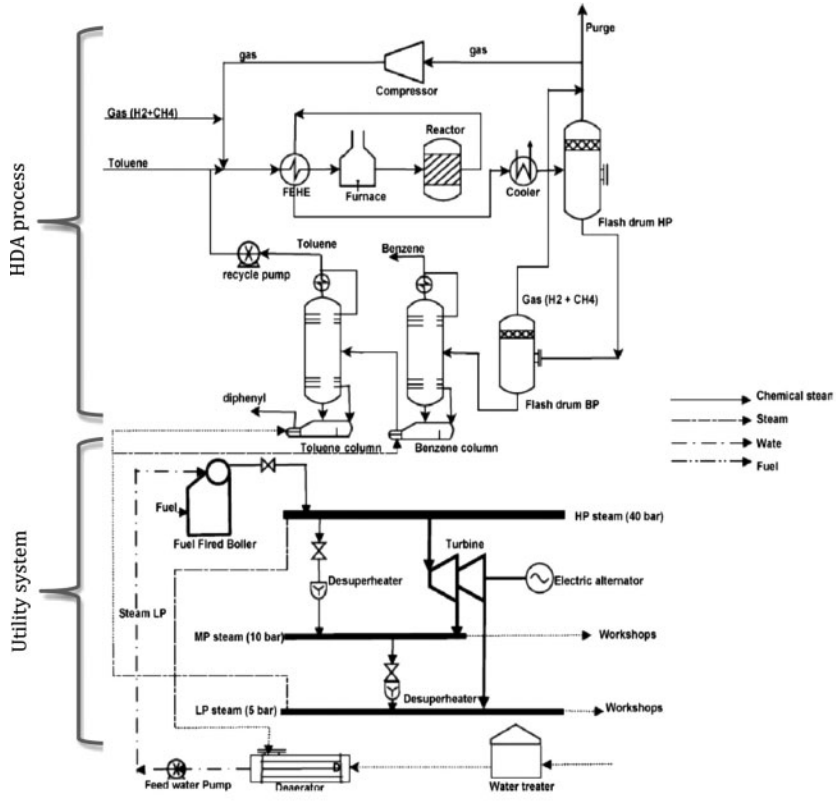

Figure 12.7 *HDA process and its associated utility system.*

The environmental impacts in some strategies like the Waste Reduction Algorithm (WAR) [35] [36], the IChemE sustainability metrics [37] [38] or the Sustainable Process Index (SPI) [39] [40] are evaluated from the environmental burdens. For a given process, the potential environmental impacts are calculated from stream mass flow rates, stream composition and emissions from utility systems and a relative potential environmental score (index) for each chemical compound can be deduced. In this study, the objective is to consider the direct impacts associated with the production of benzene together with the energy production process and its consequent emissions. The analysis therefore refers to a 'cradle-to-gate' approach. It must be emphasized that the inventory phase of extraction for the raw materials is not included to avoid counting twice their impact since our analysis is based on a process approach.

The utility system of an industrial site is of strategic importance and is generally difficult to design because a number of processes are linked to the same utility system. A typical system is proposed in this study. Three levels of steam are distributed around the site and are used by the HDA process. The HDA process has also a local fired heater for the reaction step. The primary energy requirements are computed by the use of the ARIANE^{TM} package, a decision support tool dedicated to the management of plant utilities (steam, electricity,

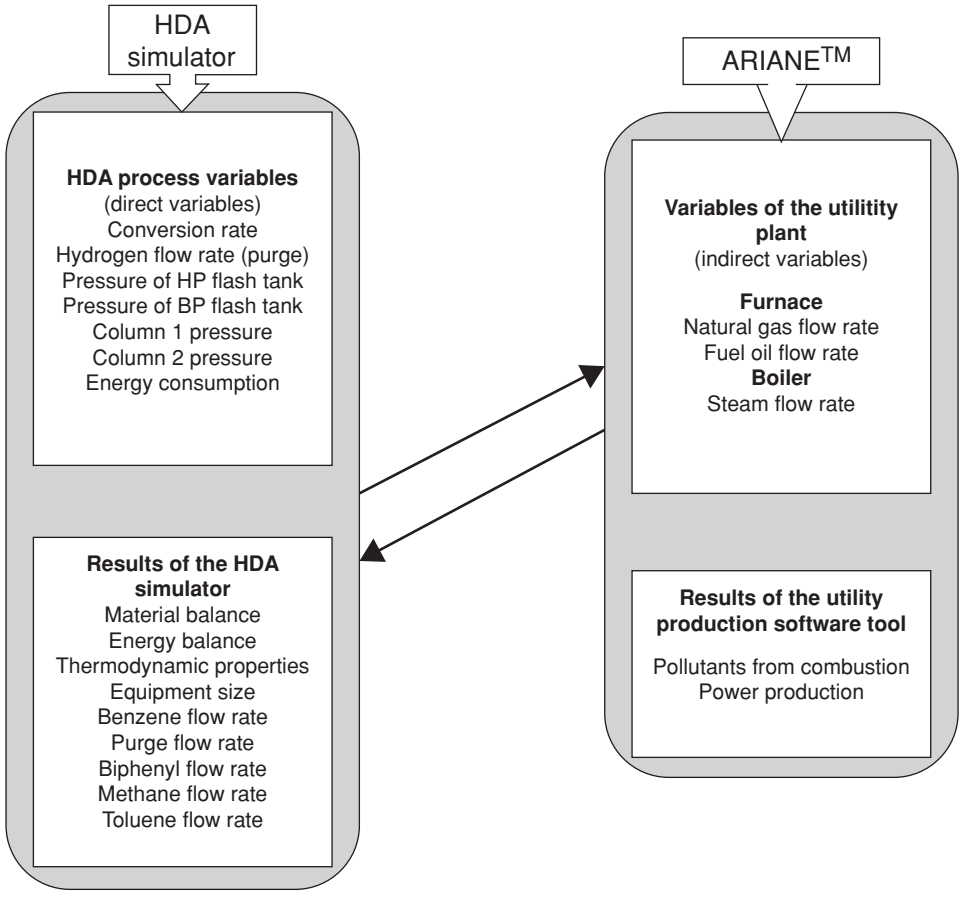

Figure 12.8 *Interaction between variables and simulation tools.*

hot water . . .). This tool is also implemented to quantify the pollutant emissions (CO_2, SO_2, NO, etc.), due to energy production. This energy production system, coupled with the HDA process, is described in Figure 12.7.

12.4.2 Optimization Variables

From the studies of Douglas (1988) [31] and Turton *et al.* (2009) [41] and due to their influence on the economic and environmental criteria, seven variables were chosen for optimizing the HDA process. They are first used to establish the overall material balance of the various chemical compounds as well as the associated thermodynamic properties (enthalpy, density, heat capacity, and so forth) at process nodes, with use of the calculation server of thermodynamic properties Simulis® Thermodynamics [42]. Then they are used to design all equipment items for carrying out the required unit operations. Figure 12.8 shows the interaction between the variables of the HDA process and the utility production system. Operation of the HDA process requires both thermal and electrical utilities. The thermal

demand is expressed in terms of fuel-flow rate to meet the need of heating the mixture in the furnace as well as of steam to meet the heating demands for the exchangers, reboilers and other process elements. These requirements obtained from the energy balances given by the HDA simulator are given to Ariane™ as shown in Figure 12.8. Then, the fuel oil flow rate, the natural gas flow rate and steam flow rate become secondary variables for Ariane™, which returns typical results concerning the thermal power plant – the power produced by the turbine and the flow rates of all the pollutants resulting from fuel combustion.

The furnace modelling is carried out by considering it as a bi-fuel reboiler fed with both natural gas and fuel oil. Their flow rates are linked by the so-called energetic ratio and the furnace energetic demand. The consumed natural gas flow rate in the furnace is calculated as follows:

$$\dot{m}_{NG} = \frac{Q_{Furnace}}{\eta \cdot LHV_{NG} \cdot ratio} \tag{12.20}$$

The consumed fuel oil flow rate in the furnace is equal to:

$$\dot{m}_{FO} = \frac{Q_{Furnace}}{\eta \cdot LHV_{FO} \cdot (1 - ratio)} \tag{12.21}$$

The energetic ratio is expressed by:

$$ratio = \frac{Energy\ provided\ by\ natural\ gas}{Total\ energy\ of\ natural\ gas\ and\ fuel\ oil|} \tag{12.22}$$

The mono-fuel reboiler is used to produce on the one hand superheated vapour, for the operation of the turbine and on the other hand, hot water for the other units.

$$\dot{m}_{NG} = \frac{Q_{Boiler}}{\eta \cdot LHV_{NG}.} \tag{12.23}$$

A reboiler is used to generate high level of pressure and temperature steam, and then this steam is expanded through a backpressure and condensing turbine to produce power. The turbine is modelled according to the formalism implemented in ARIANE™.

12.4.3 Objective Functions

12.4.3.1 Economic Assessment

In this section, a brief description is provided of economic assessments for the cost and profitability analysis that was applied. A number of books dealing with cost and profitability assessment in detail appear in chemical engineering field—for instance Peters *et al.* (2003) [43]. In this study, the retained objectives are the benzene production (*ProdB*) to be maximized and the annual cost (*Annual cost*) to be minimized. The benzene production is computed by the HDA process simulator, while the annual cost is deduced from relations (12.24) to (12.27).

$$Annual\ Cost = 0.1FCI + C_{RM} + C_{UT} \tag{12.24}$$

FCI: fixed capital investment ($).

FCI: Depreciation cost ($/y) : although there are several methods to compute depreciation, the simple straight-line method which allocates the same amount of money to every year of the recovery period, i.e. 10 years, is adopted here.

C_{RM}: Cost of raw materials (\$/y).
C_{UT}: Cost of utilities (\$/y).

The equipment cost provides the basis for the capital cost estimation and is classically expressed in terms of the main characteristics of the plant unit.

$$FCI = \sum_i (Purchase\ \cos t_i + Installed\ \cos t_i) \tag{12.25}$$

$$C_{RM} = \sum_i \dot{m}\, RMi\ P_{RMi} \tag{12.26}$$

$$C_{UT} = \sum_i \dot{m}\, UTi\ P_{UTi} \tag{12.27}$$

$\dot{m}_{RMi}$: Mass flow rate of raw material i (kg/h).
P_{RMi} : Unit price of raw material i (\$/kg).
$\dot{m}_{UTi}$: Flow rate of utility i (kg/h, std m^3/h, m^3/h or kW).
P_{UTi} : Unit price of raw material i (\$/kg, \$/std m^3, \$/m^3 or \$/kWh).

Classical Guthrie's correlations (1969) (see Table 12.7) [44] were used for computing the purchase and installed costs of the main equipment items. For the utility system, capital cost estimation was carried out by means of expressions given in [45] (see Table 12.8). Finally, the costs of raw materials and utilities obtained from Turton *et al.* (2009) [41] are reported in Table 12.9. The consumption of raw materials is given by the material and energy balances for the process. For convenience, the annual cost is expressed in M\$/y in what follows.

Table 12.7 *Capital cost estimation for main items (*M&S*: Marshall & Swift Equipment Cost (Index = 1468.6 (2009)) from* Chemical Engineering*, January 2010.*

Equipment Investment cost (\$)	Nonlinear form
Column cost D: column diameter (m) H: column height (m) F_c: material pressure F'_c: material, tray space, tray type	Purchase cost $= 9.201\left(\frac{M\&S}{280}\right)(101.9D^{1.066}H^{0.802}F_c)$ Installed cost $= 9.202\left(\frac{M\&S}{280}\right)D^{1.066}H^{0.802}(2.18+F_c) + 20.69\left(\frac{M\&S}{280}\right)4.7D^{1.55}HF'_c$
Exchanger cost A: heat exchanger area (m^2)	Purchase cost $= \left(\frac{M\&S}{280}\right)(474.7A^{0.65}F_c)$ Installed cost $= \left(\frac{M\&S}{280}\right)(474.7A^{0.65})\,(2.29+F_c)$
Furnace cost Q: furnace absorbed power (293 kW)	Purchase cost $= \left(\frac{M\&S}{280}\right)(5.52\times10^3)Q^{0.85}F_c$ Installed cost $= \left(\frac{M\&S}{280}\right)(5.52\times10^3)Q^{0.85}\,(1.27+F_c)$

Table 12.8 *Capital cost for the utility system.*

Equipment investment cost (1,000 $)	Nonlinear form
Field erected reboiler	
F: steam flow rate (kg/s);	$8.09\ F^{0.82}\ f_{p1}$
P: pressure (bar)	*With,* f_{p1}=0.6939+0.01241P-3.7984Exp(-3P^2)
Steam turbine	
W_{st}: power (MW)	$25.79W_{st}^{0.41}$
Deaerator	
F: BFW flow rate (kg/s)	$0.41F^{0.62}$
Condenser	
Q: heat dissipated (MW)	$4.76Q^{0.68}$

12.4.3.2 Environmental Assessment

Many methods for environmental assessment have been published (e.g. the so-called WAR algorithm [46] [47]). The purpose of the environmental assessment is to identify the environmental 'hot spots' in the process, meaning that special attention must be paid to those materials or steps causing most of the potential environmental burdens. The method was developed to be applied from early stages of the process development, so these environmental burdens can be significantly reduced from the beginning. Thus, the process is designed in a more sustainable way and end-of-pipe costs and consequent regulatory penalties can be avoided, or at least decreased. If there is a particular substantial environmental problem that cannot be solved, the goal of the multi-objective strategy is to identify it as soon as possible.

The environmental burden (EB), due to the emission of a range of substances, is obtained by adding the weighted emissions of each substance. The potential factor of the impact is identified as the impact factor of each substance. Let us note that a substance may contribute to different environmental burdens and may have different impact factors.

Table 12.9 *Cost of raw materials and utilities used in HDA process.*

Raw materials and utilities	Cost
Toluene	0.648 ($/kg)
Hydrogen	1.0 $/kg
Fuel oil	$549/$m^3$
Natural gas	$0.42/std m^3
Electricity	$0.06/kWh
High pressure steam	$29.97/1000 kg
Medium pressure steam	$28.31/1000 kg
Low pressure steam	$27.70/1000 kg
Cooling water (30 °C to 40 °C)	$14.8/1000 m^3

An environmental burden EB_i is computed as:

$$EB_i = \sum_{j=1}^{n} ec_i^j B_j \tag{12.28}$$

where ec_i^j is the impact potential factor of the substance j related to the environmental burden i and B_j is the amount (mass unit) of the emitted substance j. Environmental burdens are determined with respect to a reference substance (for instance SO_2 for atmospheric acidification).

From previous studies on the environmental burdens generated by the HDA process, the five following categories have been taken into account:

- Global warming potential (GWP in t CO_2 equivalent/y).
- Acidification potential (AP in t SO_2 equivalent/y) dealing with the contributions of SO_2 and NO_x to potential acid deposition—on their potential to produce H^+ protons.
- Photochemical ozone creation potential (POCP in t C_2H_4 equivalent/y) (or PCOP), known as summer smog in popular language, is the result of reactions occurring between nitrogen oxides NO_x and VOCs exposed to UV radiations.
- Human toxicity potential (HTP in t C_6H_6-equivalent/y) expresses the potential harm of chemicals released into the environment. It includes both inherent toxicity and generic source-to-dose relationships for pollutant emissions. It uses a margin-to-exposure ratio to evaluate the potential for health impact from exposure to harmful agents, including both carcinogens and noncarcinogens effects. It involves release of human toxic materials into three different media, air, water and soil.
- Eutrophication Potential (EP in t PO_4^{3-} equivalent/y) is the potential of nutrients to cause overfertilization of water and soil, which in turn can result in an increased growth of biomass.

The impact potential factors considered for the HDA case are presented in Table 12.10. As benzene is the required product, however, no associated impact has been considered in the computations.

Table 12.10 *Impact potential factors for the different impacts considered in the case of HDA.*

	HTP	EP	GWP	ODP	POCP	AP
Hydrogen	0	0	0	0	0	0
Methane	0	0	21	0	0.034	0
Benzene[a]	1	0	0	0	0.334	0
Toluene	0	0	0	0	0.771	0
Diphenyl	3.2	1.67	0	0	0	0
CO_2	0	0	1	0	0	0
SO_2	0	0	0	0	0.048	1
CO	0	0	3	0	0.027	0
NO_x	0.7	0.13	40	0	0.028	0.7
Dust	0	0	11	0	0.5	0

[a] Final product, the impact is not considered.

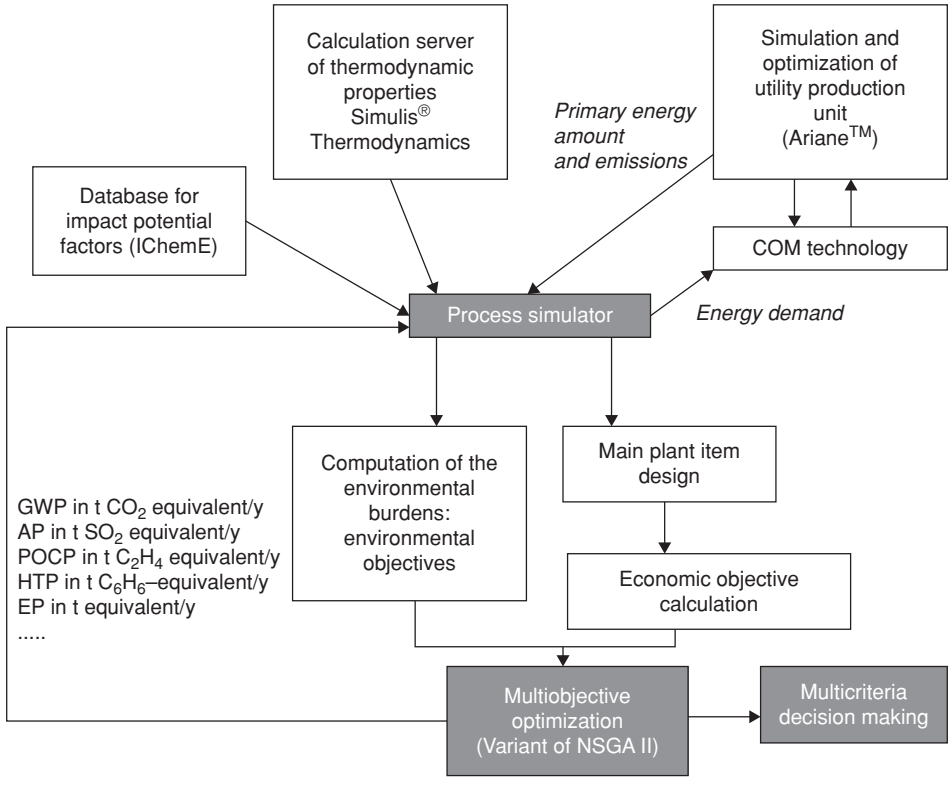

Figure 12.9 *General framework of the simulation-optimization-MCDM architecture.*

12.4.4 Multi-Objective Optimization

12.4.4.1 Ecodesign Framework

The general structure of the ecodesign assessment method is displayed in Figure 12.9.

12.4.4.2 Multi-Objective Optimization with NSGA II

In its more general form and using the previous economic and environmental objective functions defined above, the following multi-objective nonlinear optimization problem related to the HDA process ecodesign, is formulated as follows:

Determine decision variables (process operating conditions) in order to:

$$\textit{Minimize}\ (\text{annual cost}) \tag{12.29}$$

$$\textit{Minimize}\ \ (\mathrm{EB_i})\,,\ \mathrm{i} = 1,\ 5 \tag{12.30}$$

$$s.t.$$

$$\textit{Mass and energy balances (Excel}^{\circledR}\textit{and ARIANE}^{\mathrm{TM}}\textit{)}$$

Bounds on decision variables: the additional bounding constraints have been introduced in the Multigen interface, the numerical values come from the studies of Douglas (1988) [31] and Turton *et al.* (2009) [41].

- The lower bound on the benzene product is fixed at 99.97%.
- The hydrogen feed purity is assumed to be of 95%.
- The upper bound on the reactor outlet temperature is 704.50 °C.
- The quencher outlet temperature cannot exceed 621.16 °C.
- The conversion rate C lies in the range [0.5, 0.9].
- The hydrogen flow rate purged (kmol/h) is bounded between 30 and 300.
- Positive values are assumed for all pollutants, CO_2, NO_x, CO, SO_2 and dusts flow rate (kg/h).

As in the previous case study, presented in the first part of this chapter, the optimization procedure implements a multi-objective optimization genetic algorithm involving a variant of the classical NSGA II algorithm. The numerical values of the main parameters are as follows: population size = 200, number of generations = 200, crossover rate = 0.75 and mutation rate = 0.2. Douglas (1988) [31] and later Turton *et al.* (2009) [41] have defined bounds on the HDA variables (see Table 12.11). The initial population was randomly generated according to these bounds, and a randomly chosen set of variables has been extracted from the initial population for further comparison purposes (solution I in Table 12.12).

A preliminary study on the redundancy of objective was performed in [48]. In what follows, the production of benzene was set at 300 kmol/h, as justified in [47]. It was demonstrated in this study that the environmental impacts GWP, HTP and POCP can be expressed in terms of annual cost, EP and AP. From 200 randomly generated values of the independent variables, all six objectives were computed and multilinear regressions were carried out between annual cost, EP and AP as independent terms, and GWP, HTP and POCP as dependent ones. In all cases, the correlation coefficients were very good. So environmental impacts GWP, POCP and HTP being explicit functions of the annual cost, EP and AP objectives, they can be suppressed from the following multi-objective optimization phase, which is reduced to a three criteria optimization problem. A further analysis of coefficients of the multilinear equations shows that GWP and POCP are mainly increasing functions of annual cost, while HTP depends principally on EP.

Table 12.11 *Decision variables for the HDA process.*

Decision variables	Lower bound	Initial value	Upper bound
Conversion rate (%)	0.5	0.75	0.9
Hydrogen purge flow rate (kmol/h)	31	198	308
Flash pressure (bar)	30	34	34
Stabilization column pressure (bar)	4	10	10
Column 1 pressure (bar)	2	2	4
Column 2 pressure (bar)	1	1	2
Ratio (bi-fuel furnace) (%)	0.1	0.85	0.9

Table 12.12 *MCDM analysis with TOPSIS and FUCA: gain vs. the initial solution.*

Solutions	Benzene production (kmol/h)	Annual cost M$/y	EP t eq. $P0_4^{3-}$/y	AP t eq SO_2/y	GWP t eq CO_2 /y	HTP t eq C_6H_6/y	POCP t eq C_2H_4/y
Initial solution	305	277.42	9759.06	11 190.34	1 884 528.48	18 699.58	2472.32
TT1	300	205.33	13 954.31	4759.13	1 408 841.5	26 737.66	1940.78
Gain-I (%)	1.64	25.99	–42.99	57.47	25.24	–42.99	21.50
TT2	300	205.32	13 671.82	4792.25	1 410 408.66	26 196.37	1942.5
Gain-I (%)	1.64	25.99	–40.09	57.18	25.16	–40.09	21.43
TF1	300	207	9770.38	4930.16	1 428 118.43	18 720.83	1939.25
Gain-I (%)	1.64	25.38	–0.12	55.94	24.22	–0.11	21.56
TF2	300	209.03	10 109.41	4782.53	1 432 472.39	19 370.44	1928.71

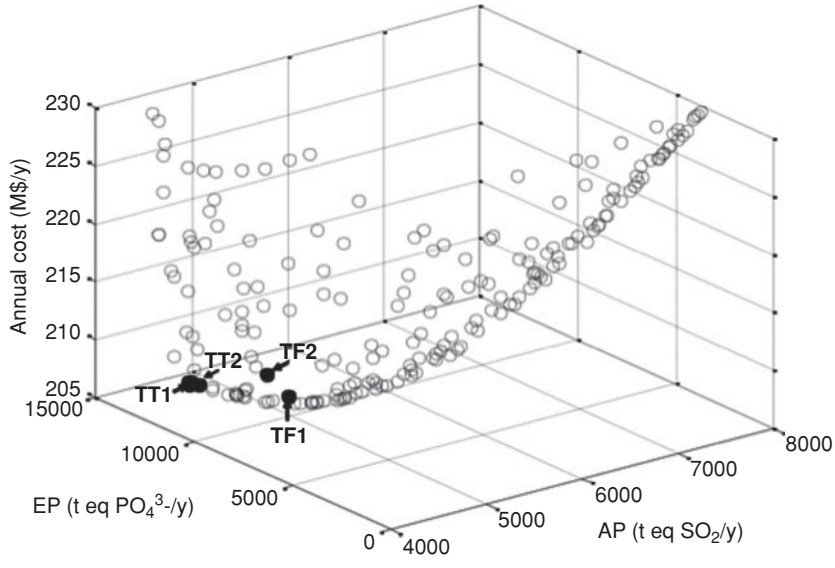

Figure 12.10 *Tri-objective optimization (*Annual cost*,* EP*,* AP*).*

12.4.4.3 Tri-Objective Optimization

Only three independent objectives remain for the multi-objective optimization phase: annual cost, EP and AP. They are now simultaneously optimized, and the results are displayed in Figure 12.10. For each set of decision variables generated by the genetic algorithm, the values of the dependent environmental criteria are also computed. It must be emphasized that two MCDM methods, namely TOPSIS and FUCA, are used after the optimization phase.

'FUCA' is the French acronym for 'Faire Un Choix Adéquat' (Making An Adequate Choice). The method relies on individual rankings of objectives; for a given criterion, rank one is assigned to its best value and rank n (n being the number of points of the Pareto front) to the worst one. Then, for each point on the front, a weighted summation (the weights representing the preferences of the decision maker) of ranks is carried out, and the choice is performed according to the lowest values of the weighted sum. Recently, the good performance of the FUCA method was established [49] by comparing it with classical engineering MCDM procedures (TOPSIS, ELECTRE, PROMETHEE). In the MCDM phase, all the criteria, either dependent or independent, are taken into account since they can influence decision-making. Only the independent criteria are represented in Figure 12.10.

In this study, the ranking was performed with the same weight assigned to each objective. The two best solutions obtained with TOPSIS (respectively FUCA) are named TT1 and TT2 (respectively TF1 and TF2) in the 3D curve (TT for Tricriterion-TOPSIS and TF for Tricriterion-FUCA). All the solutions are located in the same region of the 3D Pareto front. Tables 12.12 to 12.14 present the results obtained for the whole set of independent and dependent criteria. For each objective, the gain is expressed in percentage terms (%)

Table 12.13 *MCDM analysis with TOPSIS and FUCA: gain versus the economic solution.*

Solutions	Benzene production (kmol/h)	Annual cost M$/y	EP t eq. $P0_4^{3-}$/y	AP t eq SO_2/y	GWP t eq CO_2 /y	HTP t eq C_6H_6/y	POCP t eq C_2H_4/y
Economic solution	299.76	205.04	13 831.12	4829.26	1 410 428.13	26 537.88	1944.11
TT1	300	205.33	13 954.31	4759.13	1408,841.5	26 737.66	1940.78
Gain-E (%)	–0.08	–0.14	–0.89	1.45	0.11	–0.75	0.17
TT2	300	205.32	13 671.82	4792.25	1 410 408.66	26 196.37	1942.5
Gain-E (%)	–0.08	–0.13	1.15	0.77	0	1.29	0.08
TF1	300	207	9770.38	4930.16	1 428 118.43	18 720.83	1939.25
Gain-E (%)	–0.08	–0.95	29.36	–2.09	–1.25	29.46	0.25
TF2	300	209.03	10 109.41	4782.53	1 432 472.39	19 370.44	1928.71
Gain-E (%)	–0.08	–1.95	26.91	0.97	–1.56	27.01	0.79

Table 12.14 *MCDM analysis with TOPSIS and FUCA: gain versus the Douglas solution.*

Solutions	Benzene production (kmol/h)	Annual cost M$/y	EP t eq. $P0_4^{3-}$/y	AP t eq SO_2/y	GWP t eq CO_2 /y	HTP t eq C_6H_6/y	POCP t eq C_2H_4/y
Douglas solution	300	327	9759.13	14 777.59	2 175 734.97	18 699.58	2794.30
TT1	300	205.33	13 954.31	4759.13	1 408 841.5	26 737.66	1940.78
Gain-D (%)	0	37.21	–42.98	67.79	35.25	–42.99	30.55
TT2	300	205.32	13671.82	4792.25	1 410 408.66	26 196.37	1942.5
Gain-D (%)	0	37.21	–40.09	67.57	35.18	–40.09	30.48
TF1	300	207	9770.38	4930.16	1 428 118.43	18 720.83	1939.25
Gain-D (%)	0	36.70	–0.12	66.64	34.36	–0.11	30.60
TF2	300	209.03	10 109.41	4782.53	1 432 472.39	19 370.44	1928.71
Gain-D (%)	0	36.08	–3.59	67.64	34.16	–3.59	30.98

Table 12.15 *Decision variables corresponding to solutions TT1, TT2, TF1, TF2 and Douglas.*

Decision variables	TT1	TT2	TF1	TF2	Douglas
Toluene conversion rate	0.80	0.79	0.75	0.76	0.75
Hydrogen flow rate at the purge (kmol/h)	300	300	300	300	198
Flash pressure HP (bar)	33.98	33.94	33.94	33.89	34.45
Flash pressure BP (bar)	9.96	10	9.66	9.97	10.33
Column 1 pressure 1 (bar)	3	3	3	3	1.034
Column 2 pressure 2 (bar)	1.15	1.71	1.13	1.02	1.034

(denoted as Gain-I and, Gain-E and Gain-D respectively) relative to a reference solution that can be: (i) a solution randomly chosen in the initial population of the GA, referred to as solution I for initial; (ii) one obtained from a single objective optimization based on the economic criterion, referred to as solution E for economic; (iii) the solution corresponding to the conditions of Douglas (1988) [31] with the production adopted in this study (i.e., 300 kmol/y) to be consistent, referred to as solution D [34]. The values corresponding to these solutions are reported in Table 12.15.

The results show that the global gain for all the objectives is higher with FUCA. A closer look at solutions TF1 and TF2 leads to the final selection of TF2 because it gives only one negative gain over all the environmental impacts, which corresponds to a degradation of 1.95% of the annual cost. The values of the optimization variables corresponding to solutions TT1, TT2, TF1 and TF2 are compared to the solution obtained by Douglas (1988) [31] in Table 12.15. The corresponding design is proposed in Table 12.16.

A radar chart (Figure 12.11) is also proposed to compare the solutions with the reference ones. All the values are normalized to make easier the representation, by dividing each value by its maximal one.

Information can be obtained about environmental impacts generated by the various unit operations. They are represented in Figure 12.12 for the TF2 and Douglas solutions. The

Table 12.16 *Design variables corresponding to solutions TT1, TT2, TF1, TF2 and Douglas.*

Equipment	TT1	TT2	TF1	TF2	Douglas
Furnace power (GJ/h)	93.12	93.35	98.41	97.77	121.46
Volume of the reactor (m^3)	173.32	173.03	170.29	170.39	251.61
Flash HP : volume (m^3)	22.86	22.97	24.83	24.62	38.65
Flash BP: volume (m^3)	2.26	2.25	2.50	2.42	2.93
Column 1 : height (m)	42.37	42.37	42.98	42.98	36.88
diameter (m)	2.89	2.89	2.93	2.93	3.68
Column 2 : height (m)	17.98	18.59	17.98	17.98	17.98
diameter (m)	1.66	1.54	1.88	1.89	1.91
Heat exchanger B : exchange surface(m^2)	525.91	527.13	554.44	550.97	668.72
Power compressor (kW)	100.00	100.30	107.07	106.21	145.10
Pump power (kW)	2.50	2.50	2.63	2.61	2.63
Recycling pump power (kW)	11.05	11.04	14.53	14.18	14.58

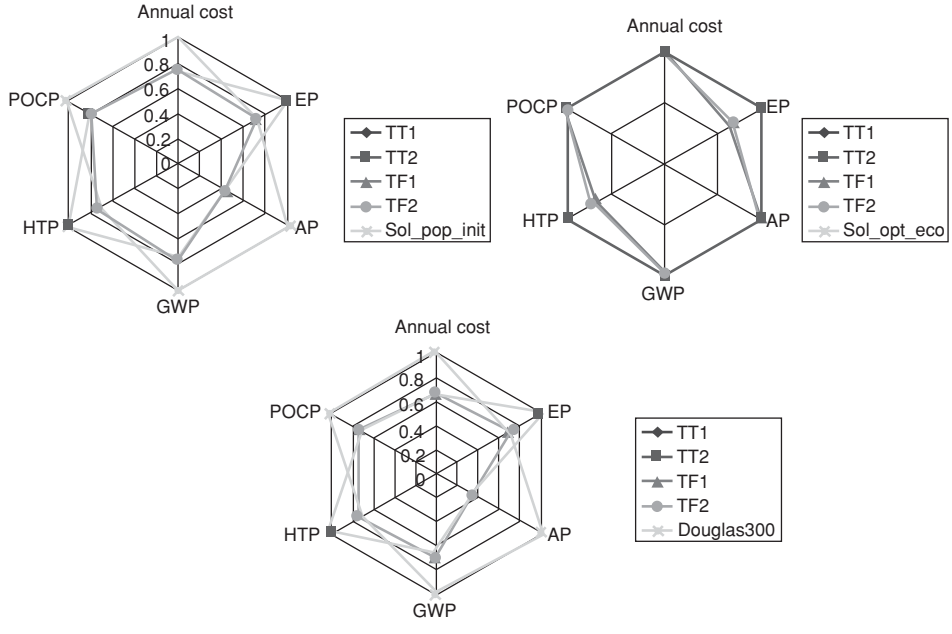

Figure 12.11 *Radar charts corresponding to solutions TT1, TT2, TF1, TF2, initial, economic and Douglas solutions.*

impacts of HTP and EB are mainly due to the output of column 2, because they are caused by the emissions of diphenyl by the HDA process. Methane at the purge contributes significantly to the high value of GWP. The very important value of GWP computed for tye Douglas solution can be attributed to the assumption made concerning furnace modeling that uses only fuel. This is a penalizing hypothesis that was not specified in the work of Douglas (1988) [31] but is made here to show how the choice of an energy solution can be detrimental to environmental performances.

By using this simplified assessment method, decision making based on a multi-objective optimization strategy and multicriteria decision making can help in the search for a good solution at the early stages of a process design phase. This method can identify the 'hot spots' of the system and concentrates on the process and its associated energy production unit. To be more precise, as far as the resource extraction phase is concerned and to perform inventory more accurately, other methods relevant to the life–cycle assessment field must be applied and may help to a certain extent. However, such methods are time-consuming, particularly with regard to data collection and reconciliation and can be used after this preliminary grass-root design stage.

12.5 Conclusions

This chapter presented two examples showing growing interest in using multi-objective optimization techniques at the early stages of process ecodesign. The first was the didactic

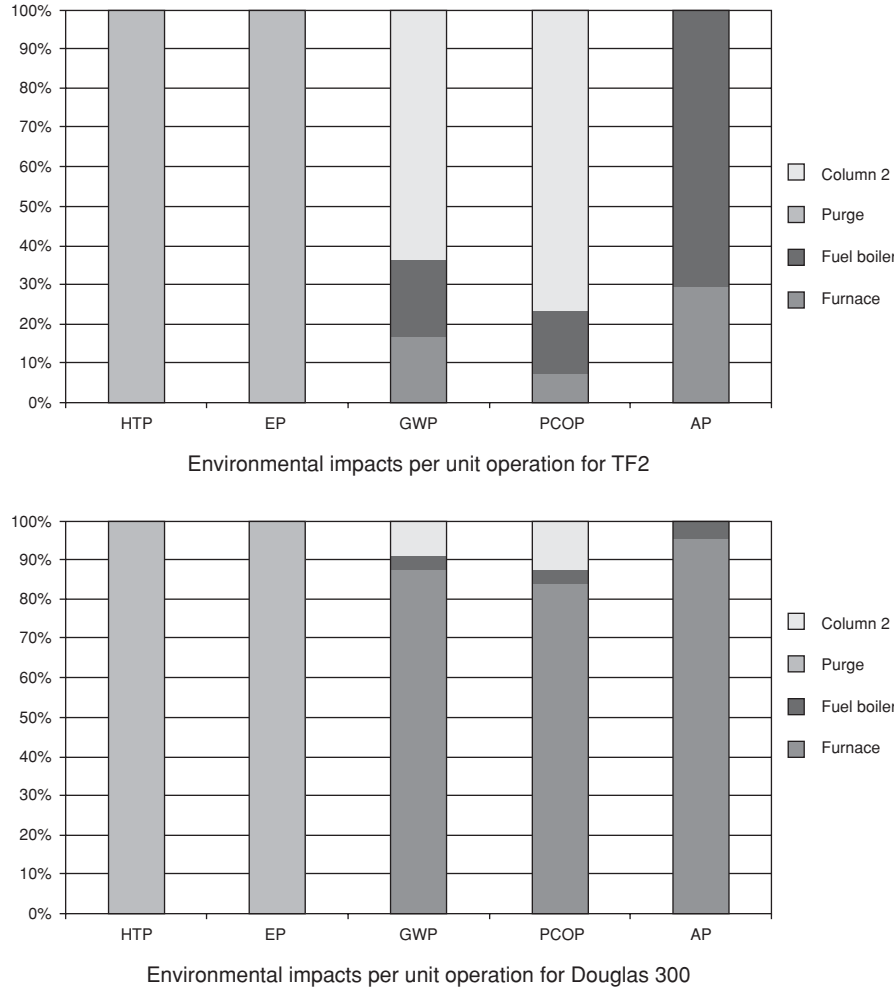

Figure 12.12 *Environmental impacts per unit operation for solutions TF2 and Douglas.*

case of the so-called Williams and Otto process revised in a tricriteria optimization mode with two economic criteria and one environmental objective, based on the minimization of a pollutant flow rate. This corresponds to a traditional approach in chemical engineering where direct waste from a process has to be minimized.

The approach was then extended to treat the combined influence of release and waste flow rates via objective functions involving indicators based on environmental impacts. For this purpose, a more general methodology was proposed for the ecodesign and optimization of a chemical process taking into account the contribution of utility generation, via the industrial software ARIANE^{TM}. This chapter outlined a systematic methodology for evaluating environmental and health-based impacts of chemical process designs. Multiple impact indexes are included for process evaluation because of the complexity of pollutant interaction with

the environment and with human health. The impacts are considered as linear functions relative to each category of the emitted substance's amount. The benchmark HDA process, first developed by Douglas (1988) [31], illustrates the approach. In many published papers, this process was optimized considering classical engineering objectives, particularly benzene production and total annual cost. The problem is revisited here also considering engineering criteria and classical environmental burdens: global warming potential, acidification potential, photochemical ozone creation potential, human toxicity potential and eutrophication potential. An upgrade version of the well-known multi-objective genetic algorithm NSGA II is implemented for solving the various multi-objective problems.

A preliminary study on the objectives was performed for identifying a subset of dependent criteria (GWP, POCP and HTP) expressed as multilinear functions in terms of the three remaining independent ones (annual cost, AP and EP). In that way, the multi-objective problem was reduced to a tri-criteria one. This reduction of the number of objectives can be applied to a wide spectrum of design problems in chemical engineering, involving multiple and environmental objectives and makes explicit the tradeoffs between them.

During the tri-objective optimization phase, the values of the dependent objectives were computed for each set of independent variables generated by the genetic algorithm, and MCDM analyses based on TOPSIS and FUCA were carried out on the whole set of objectives.

Finally, multi-objective optimization alone or combined with MCDM methods constitutes an interesting framework to integrate green engineering concepts into process synthesis and design. The areas of green engineering represent a balance between several competing objectives. A promising theory for the integration of green engineering and sustainability principles in the process optimization is the inclusion of sustainability and life-cycle assessment metrics into the design using a life cycle framework in the formulation of multi-objective design and synthesis for chemical plants.

Another issue to consider is the uncertainties involved in the assessment of environmental risk. It is important to study whether the order of magnitude of the uncertainty associated with the evaluation of the various impacts is quite different and how it can influence process operating conditions and the choice of process technologies. Uncertainty analysis for environmental impact assessment is an active research area that has now to be integrated into multi-objective optimization and multiple criteria decision making for process design. Fuzzy concepts, Monte Carlo simulation and propagation of error analyses are possible ways to address the uncertainties in environmental assessment for process ecodesign.

Acronyms

AP	atmospheric acidification potential (eq t SO_2/y).
EB_i	i^{th} environmental burden.
EP	eutrophication potential (eq t PO_4^{3-}/y).
FUCA	French acronym for 'Faire Un Choix Adéquat' ('Make an Adequate Choice').
GWP	global warming potential (eq t CO_2/y).
HDA	benzene production from toluene hydrodealkylation.
HTP	human toxicity potential (t C_6H_6/y).
LCA	life cycle assessement.

MCDM	multiple choice decision making.
NLP	nonlinear programming.
NPW	net present worth.
NSGA	nonsorted genetic algorithm.
PBP	pay back period.
PBT	profit before tax.
POCP	photochemical oxidation or smog formation potential (eq t C_2H_4/y).
SBX	simulated binary crossover operator.
TOPSIS	technique for order preference by similarity to ideal solution.
WAR	waste reduction algorithm.
WOP	Williams and Otto Plant.

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