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A systematic approach to the optimal design of chemical plants with waste reduction and market uncertainty

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ABSTRACT: The paper presents a methodology for the quantitative assessment of sustainability applied to the design of chemical plants. Specifically, we focus on the economic and environmental sustainability. The methodology implemented for the economic assessment is the predictive conceptual design (PCD) that uses as indicator the cumulated dynamic economic potential over a long-term horizon. PCD accounts for both CAPEX and OPEX terms, which on their turn depend on dynamic econometric models of commodities and utilities. The environmental assessment is based on the waste reduction algorithm and on the evaluation of the potential environmental impact. The benefit of PCD consists in accounting for market uncertainty and prices/costs volatility of OPEX terms. The optimal solutions of the economic and environmental assessment lay on the Pareto line produced by the multi-objective-optimization (MOO) problem. The MOO of a cumene plant allows discussing various optimal solutions in terms of economic and environmental concerns/criteria.

KEYWORDS: Economic sustainability; Environmental sustainability; Predictive conceptual design; Process design; Multi objective optimization; Pareto curve; Cumene plant.

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1 Introduction

The chemical manufacturing industry is a multinational, varied scale sector that makes plenty of products available to promote social development and economic growth (Hall and Howe, 2010). Chemical industry is one of the four major energy-intensive industries, which include iron and steel, cement, and pulp and paper (Schönsleben et al., 2010). Past global events raised the awareness that substantial changes in energy and material utilization are recommended if not necessary for the sustainability of chemical industry. For instance, the increase in crude oil (CO) prices registered for several quarters till the third quarter of 2008 drove the chemical industry to devise efficient technologies to reduce energy intensity and manufacturing costs (National Resource Council, 2005). In addition, carbon dioxide (CO₂) emissions to the atmosphere received great attention. Grossmann (2004) reported that the level of CO₂ in the atmosphere increased by a third since the beginning of the industrial age, and that CO₂ contributes more than 70% to the potential for global warming. Process design methodologies play an important role in industrial sustainability. For instance, Marechal et al. (2005) included life cycle analysis, optimization, and other computer-aided systems among the recommended research and development (R&D) priorities. In this respect, there has been a renewed interest in Process Systems Engineering (PSE), which is devoted to the development of rigorous tools and techniques for the analysis of complex systems (Grossmann and Guillén-Gosálbez, 2010). The idea of sustainability took root in the international scientific community after the publication of the "Our Common Future" book by the World Commission on Environment and Development (WCED, 1987). WCED focused on the issues of environmental degradation and social inequity that result from the wasteful consumption of natural resources, and recognized that sustainable development "*meets the needs of the present without compromising the ability of future generations to meet their own needs*". This definition allowed for various interpretations. To explain the implication of sustainability for chemical engineering, Sikdar (2003) identified four types of sustainable systems: (i) those referred to global concerns or problems, (ii) those characterized by geographical boundaries (*e.g.*, cities, villages), (iii) businesses, either localized or distributed, and (iv) any particular technology that is designed to provide economic value through clean chemistry. Systems (iii) and (iv) reduce the region of influence to product/process design and manufacturing methods, which are more suitable for chemical engineering problems. In particular, a sustainable product or process can be defined as "*the one that constraints resource consumption and waste generation to an acceptable level, makes a positive contribution to the satisfaction of human needs, and provides enduring economic value to the business enterprise*" (Bakshi and Fiksel, 2003). Consequently, a certain engineering solution must agree with social requirements, and has to be economically feasible and environmentally friendly (García-Serna et al., 2007). Actually, social sustainability is often neglected due to the lack of rigorous methods capable of accounting for it, despite the recent attempts to integrate the social aspects into the decision-making process (Simões et al. (2014); Azapagic et al. (2016)).

The combined use of sustainability assessment tools and optimization methods allows identifying those process alternatives that minimize the environmental impact while yielding good economic performance (Carvalho et al., 2008; Grossmann and Guillén-Gosálbez, 2010; Jensen et al., 2003). Several methodologies and indicators have been developed and applied to support environmental decisions (Burgess and Brennan (2001); García-Serna et al. (2007)). As far as the economic performance is concerned, most studies adopt the conventional approach to conceptual design (CD) based on the assumption of fixed prices of raw materials, (by)products, and utilities. This assumption is not representative of reality, since the price of commodities and utilities can vary significantly according to demand and offer fluctuations, and market uncertainty. As a result, price volatility has an intense influence on the economic sustainability of chemical plants. Aim of this paper is to propose an effective procedure to account for price/cost fluctuations in the

optimal design of chemical plants, and illustrate a comprehensive approach to reconcile the economic goal with the environmental concern. This paper considers as a case study the cumene process (Pathak et al., 2011), which provides an interesting example of plantwide design optimization subject to some classical engineering trade-offs (Luyben, 2010).

2 Methodology

As shown in Figure 1, the modeling and optimization approach used in this paper goes through a sequence of steps. Once the process to be studied has been selected, the plant simulation is configured to assess both the economic and environmental impacts. Eventually, a multi-objective optimization (MOO) evaluates the trade-offs between the competing targets of economic and environmental sustainability. Outcome of this procedure is the identification of the optimal design configuration for equipment size and nominal operating conditions.

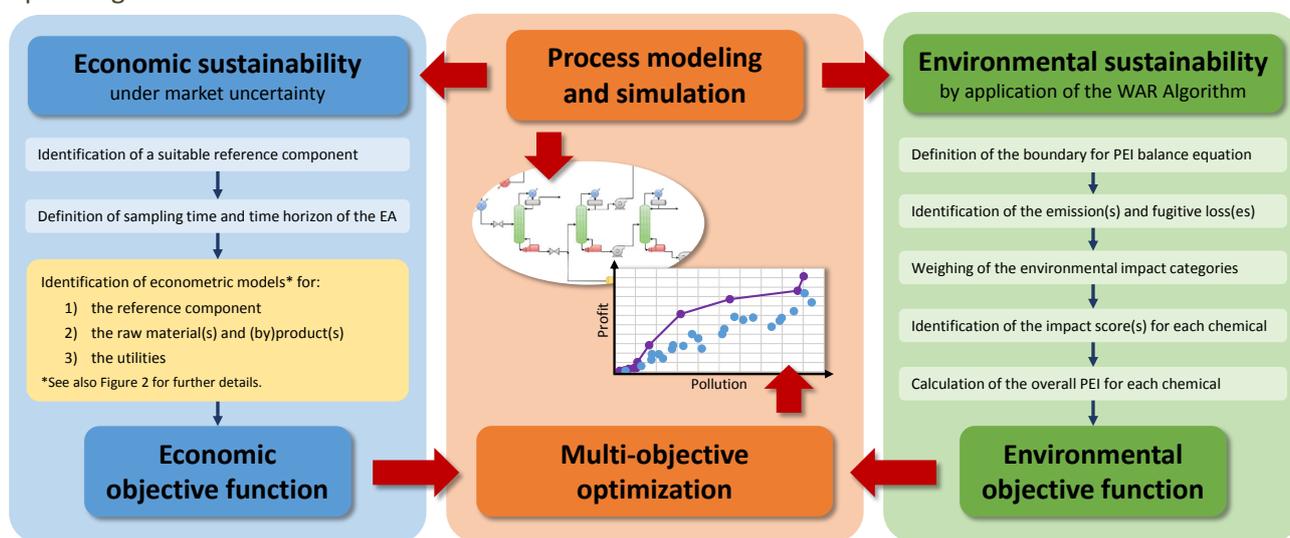


Figure 1: Systematic approach to the optimal design of sustainable chemical plants.

2.1 Economic sustainability

The methodology for the assessment of economic sustainability lies on the evolution of conventional CD. Douglas (1988) proposed a hierarchical approach to the CD of industrial plants based on both operative expenditures (OPEX, *i.e.* the costs associated to running the plant) and capital expenditures (CAPEX, *i.e.* the cost associated to equipment purchase/setup). This hierarchical approach goes through a series of decision levels grounded on suitable economic potentials (EPs). Each EP (Douglas defined four EPs out of a sequence of five decision levels) progressively calls for a more in-depth analysis of the CAPEX and OPEX terms in each section of the plant (*i.e.* input-output boundaries, recycles, reaction and separation sections, and heat-exchanger network). The plant is economically attractive if the EPs are positive. Douglas (1988) assumed that the prices/costs of commodities and utilities, which characterize the OPEX terms throughout the lifetime of the plant, are fixed (*i.e.* time invariant). This is a quite substantial limitation for the economic assessment (EA) of industrial plants, as market fluctuations play a primary role in making uncertain the future feasibility of the designed plant. Indeed, prices/costs of raw materials and products can oscillate and make the plant production either profitable or unprofitable as a function of their relative volatility. For instance, Manca et al. (2011) showed for the hydrodealkylation (HDA) process the continuously crossing

trends of benzene (*i.e.* the product) price and toluene (*i.e.* the raw material) cost over a long-term horizon (*i.e.* some years). Whenever the benzene price is lower than the toluene cost, the necessary condition for the economic sustainability of the process is not met, and the plant should not be operated (Milmo, 2004). Barzaghi et al. (2016) discussed the optimal design of a styrene monomer plant under market volatility, and showed that the hypothesis of fixed prices is unacceptable, as it would lead to continuously changing optimal configurations. In addition, they determined the existence of a CO quotation threshold beyond which the plant is not economically sustainable. This point is noteworthy, as in the past decade CO quotations have experienced very important oscillations with alternating bullish and bearish trends. Some considerations about physical and macroeconomic driving forces of CO volatility are reported in Manca et al. (2015), and Manca and Depetri (2016).

Manca and coauthors (Manca and Grana (2010), Manca et al. (2011), Manca (2013), Barzaghi et al. (2016)) proposed two methodologies to carry out feasibility studies of chemical plants under market uncertainty, respectively christened Dynamic Conceptual Design (DCD) and Predictive Conceptual Design (PCD). Both procedures are based on the same hierarchical approach to EPs of Douglas, but they remove the hypothesis of fixed prices for the evaluation of the economic performance, and consider the uncertainties that inevitably affect future OPEX terms and profits. However, PCD differs from DCD, as DCD optimizes the design of a plant by considering the historical price time series, while PCD uses specific econometric models (EMs) to devise a set of possible future scenarios of the price/cost of both commodities and utilities, and find an optimal plant configuration for each scenario. For the sake of conciseness, this paper tackles only the PCD methodology for the assessment of the economic sustainability of chemical plants.

The PCD procedure introduces a direct time dependency in the Eps formulation, and considers the variable profits and OPEX terms as a function of price fluctuations, which result in the definition of the Dynamic Economic Potentials (DEPs) (Manca et al., 2011). The CAPEX assessment for each process unit is performed by means of Guthrie's formulas updated with the M&S cost index (Peters et al., 2003). Guthrie's formulas estimate the purchase and installation costs of process units by considering some characteristic dimensions, materials, and operating pressures. The OPEX terms are computed by multiplying the inlet/outlet flowrates (obtained from steady-state mass and energy balances) times their corresponding prices/costs that fluctuate subject to market volatility. As far as price/cost fluctuations are concerned, Manca (2013) and Manca (2016) presented suitable EMs for both commodities and utilities that allow evaluating possible future economic scenarios over long-term horizons, and showed how Autoregressive Distributed Lag (ADL) models are suitable for PSE/CAPE applications. At once, it is useful to identify a functional dependency of commodity (*e.g.*, distillates and derived petrochemical products) and utility (*e.g.*, electric energy, fuel gas, steam) prices respect to the quotations of a reference component that plays a key role on their quotations in the specific market where the plant is operated. CO and natural gas (NG) are good candidates for the role of reference component, as they (i) are precursors of a number of (petro)chemical components, (ii) are involved as fuels in power generation plants (with different proportions in the energy mix depending on the concerned country), and (iii) their cost is well-known and largely available. Figure 2 summarizes the methodology used to identify the EMs, which are implemented in Section 3.2.

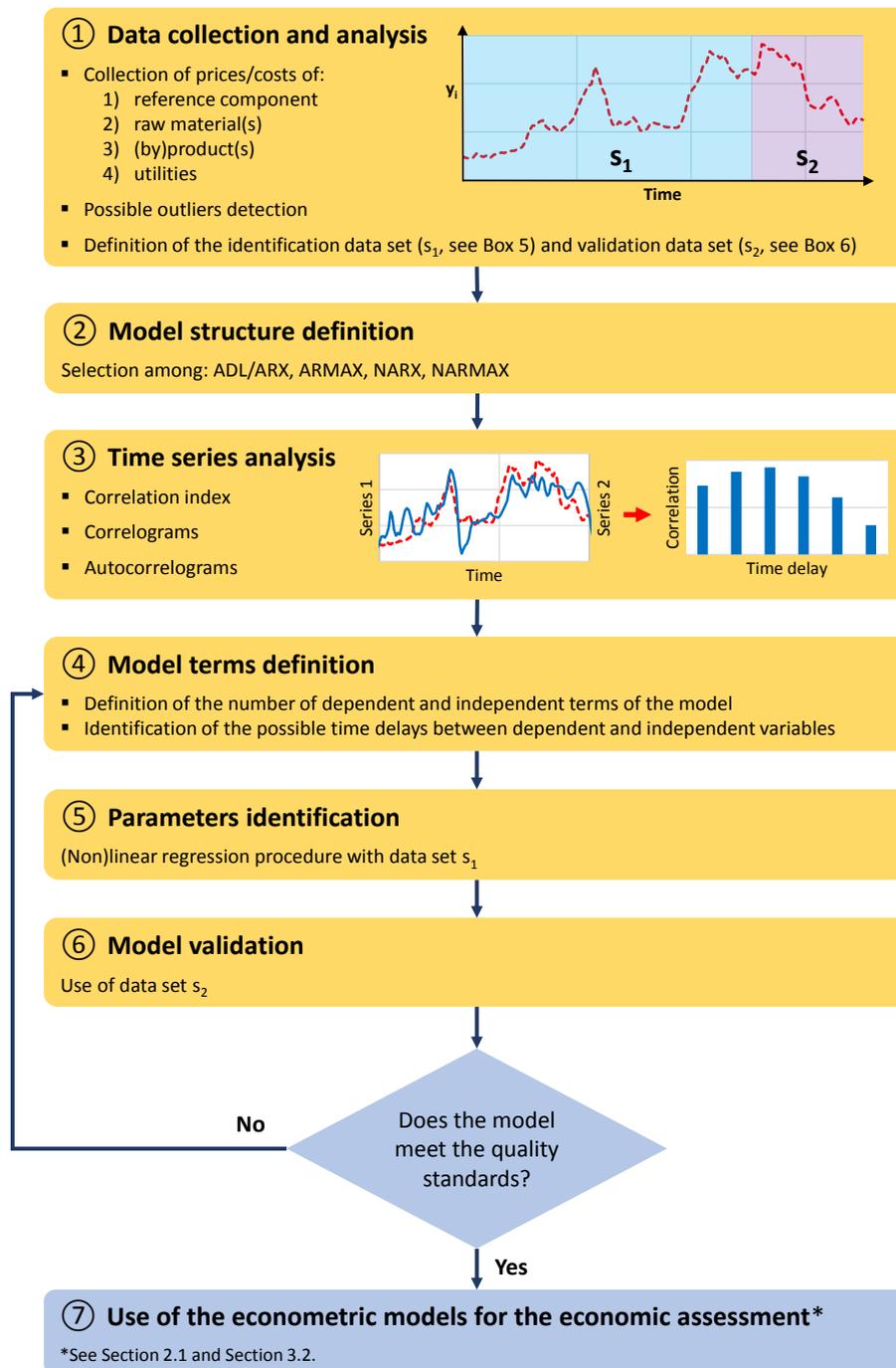


Figure 2: Methodology used to identify the EMs.

For design and sustainability assessment purposes, the typical time horizon is the expected lifetime of the plant or at least a substantial fraction of it (*i.e.* some years). This latter option is a compromise between a sufficient time horizon for forecast purposes and the reliability of the adopted EMs. Instead, the choice of a suitable sampling time depends mainly on the availability of real prices linked to the involved financial market and the complexity/detail of the numerical simulation. Manca et al. (2011) showed a systematic approach to finalize the EMs of raw materials, (by)products, and utilities that contribute to evaluate and forecast the OPEX terms. The fourth-level DEP calculated for the k -th economic scenario has the following formulation:

$$DEP4_k [USD / y] = \sum_{i=1}^N Revenues_{i,k} \cdot nHpY - \frac{CAPEX}{N / 12} \quad (1)$$

$$\text{with: } Revenues_{i,k} [USD / h] = \max \left[0, \left\{ \sum_{p=1}^{NP} C_{p,i,k} \cdot F_p - \sum_{r=1}^{NR} C_{r,i,k} \cdot F_r - OPEX_{i,k} \right\} \right]$$

where NP and NR are the number of products and reactants, respectively; C stands for the prices/costs; F_p and F_r are the flowrates of products and reactants, respectively; N measures the length of the horizon in months used for the EA; $nHpY$ is the number of production hours in a year; i and k are the subscripts for a specific month and scenario, respectively.

Cumulated DEP4 is the objective function for the economic sustainability in the PCD method. It is defined as the sum of monthly values of *DEP4* throughout the operational life span of the plant, for the k -th economic scenario:

$$(Cumulated DEP4)_k = \sum_{i=1}^N DEP4_{i,k} \quad k = 1, \dots, K \quad (2)$$

For the sake of clarity, each k -th scenario describes a possible economic trajectory of prices/costs for the assessment of both revenues and OPEX terms. This means that PCD adopts a probabilistic approach to the EA of chemical plants, from which valuable information on the distribution of expected optimal values can be extracted.

The intrinsic fluctuations of future price scenarios bring about a probabilistic distribution of the *Cumulated DEP4*, which represents the economic impact of the designed plant. Negative values of *Cumulated DEP4* mean economic losses in case of plant operation under specific economic scenarios, while positive values foreshadow plant economic sustainability. The optimal design problem searches for the plant configuration that maximizes the *Cumulated DEP4* subject to either a specific scenario or a set of scenarios (in this case the assessment becomes probabilistic). The best *Cumulated DEP4* amongst the different plant configurations outlines the optimal plant configuration (*i.e.* the optimal set of degrees of freedom). For the sake of brevity, we will provide results that are based only on one specific economic scenario, which is representative of the recent historical price/cost trends. Hence, this article does not discuss the results obtained by the probabilistic distribution of future scenarios.

2.2 Environmental sustainability

A number of methodologies are available in the literature for the characterization of the environmental impact of chemical products and processes (Burgess and Brennan (2001); García-Serna et al. (2007)). The recommended approach to the design of environmentally benign processes is to identify potential pollution problems early in the development stages rather than use end-of-pipe treatments (Douglas, 1992). For instance, Life Cycle Assessment (LCA) and the Waste Reduction (WAR) algorithm are well-established techniques to include environmental considerations into process design or retrofitting. LCA is supposed to assess the environmental performance of a product or process from the *cradle* of primary resources to the *grave* of recycling or safe disposal (Clift, 2006). The main drawback of LCA is the large amount of information required over the life cycle, and the lack of public data due to legal or intellectual property concerns (Jiménez-González et al., 2000). At the early design stage, extensive data related to process alternatives are not available, and the focus is more on excluding the worst alternatives instead of finding the best one (Diwekar and Shastri, 2011). In this respect, a data-intensive approach is not helpful, whereas the estimation of gate-to-gate information becomes feasible. The WAR algorithm considers only the

manufacturing step of the overall life cycle of a product, thus neglects raw material(s) acquisition and product(s) distribution, use, disposal, and recycle (Young et al., 2000). However, it is a simple tool to be used by design engineers to evaluate the environmental friendliness of a process (Young and Cabezas, 1999).

The WAR algorithm has been used to describe the environmental performance of unit operations (Chen and Feng (2005); Ramzan et al. (2008)), optimize chemical manufacture and recovery (Kim and Smith (2004); Shadiya et al. (2012)), design eco-efficient biodiesel processes (Couto et al. (2011); Marulanda (2012); Othman et al. (2010)), and model industrial utility systems (Idris et al., 2016). We chose to apply the WAR algorithm to evaluate the environmental impact of both the cumene production and the energy consumed within the process (see also Section 3.3). Figure 3 shows a summary of the theoretical background adopted in this article.

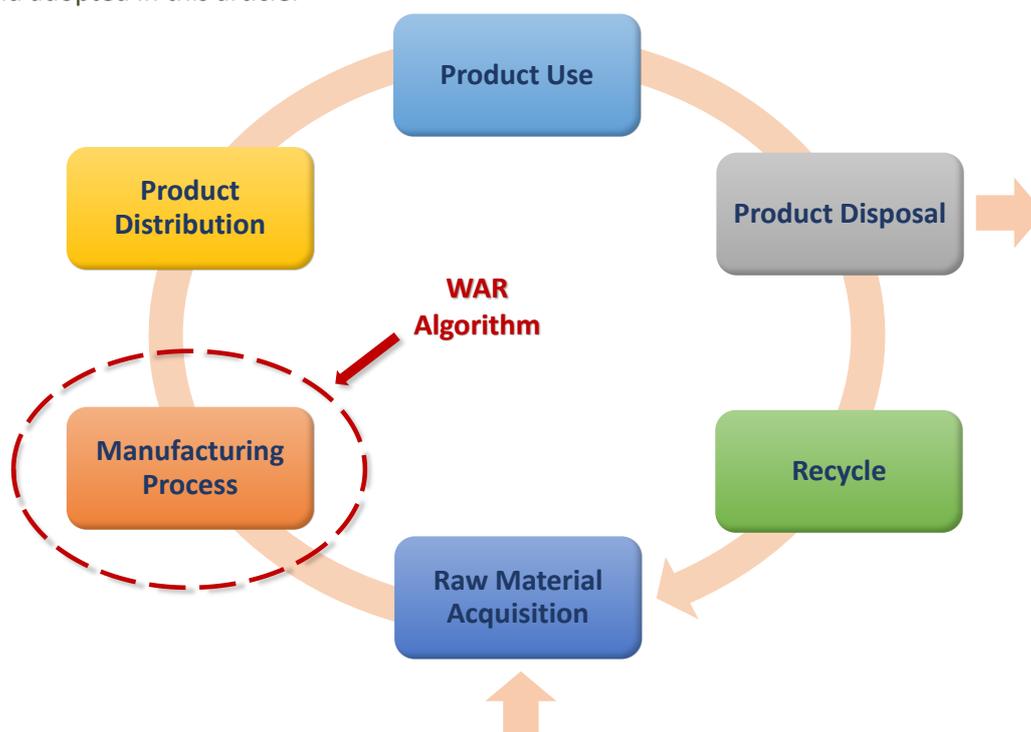


Figure 3: Applicability of the WAR algorithm to the product life cycle (adapted from Young and Cabezas (1999)).

2.2.1 Impact balance and indicators

The WAR algorithm determines the potential environmental impact (PEI) of a chemical process. The PEI of a given amount of material or energy can be defined as the effect that such an amount would have once emitted into the environment (Young and Cabezas, 1999). This implies that the PEI of a particular emission is probabilistic in nature, and an average estimate of the effect that this emission is likely to have (Young et al., 2000). Cabezas et al. (1999) proposed to consider a balance equation describing the PEI of a manufacturing process to incorporate environmental aspects into the process design. Young and Cabezas (1999) improved that balance by including the energy generation process (Figure 4). For steady state processes, the PEI balance equation is:

$$\dot{I}_{in}^{(cp)} + \dot{I}_{in}^{(ep)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} - \dot{I}_{we}^{(cp)} - \dot{I}_{we}^{(ep)} + \dot{I}_{gen}^{(syst)} = 0 \quad (3)$$

where $\dot{I}_{in}^{(cp)}$ and $\dot{I}_{out}^{(cp)}$ are the input and output PEI to the chemical process, $\dot{I}_{in}^{(ep)}$ and $\dot{I}_{out}^{(ep)}$ are the input and output PEI to the energy generation process, $\dot{I}_{we}^{(cp)}$ and $\dot{I}_{we}^{(ep)}$ are the output PEI associated with waste

energy lost by chemical and energy generation processes, and $\dot{I}_{gen}^{(syst)}$ is the rate of PEI generation by the system. As observed by Young and Cabezas (1999), chemical plants do not emit large amounts of waste energy generally, and the PEI associated with energy emission is usually negligible compared to the PEI associated with the mass emission (e.g., toxic substances, pollutants, solid/liquid/gas wastes). Therefore, Equation (3) can be simplified to:

$$\dot{I}_{in}^{(cp)} + \dot{I}_{in}^{(ep)} - \dot{I}_{out}^{(cp)} - \dot{I}_{out}^{(ep)} + \dot{I}_{gen}^{(syst)} = 0 \quad (4)$$

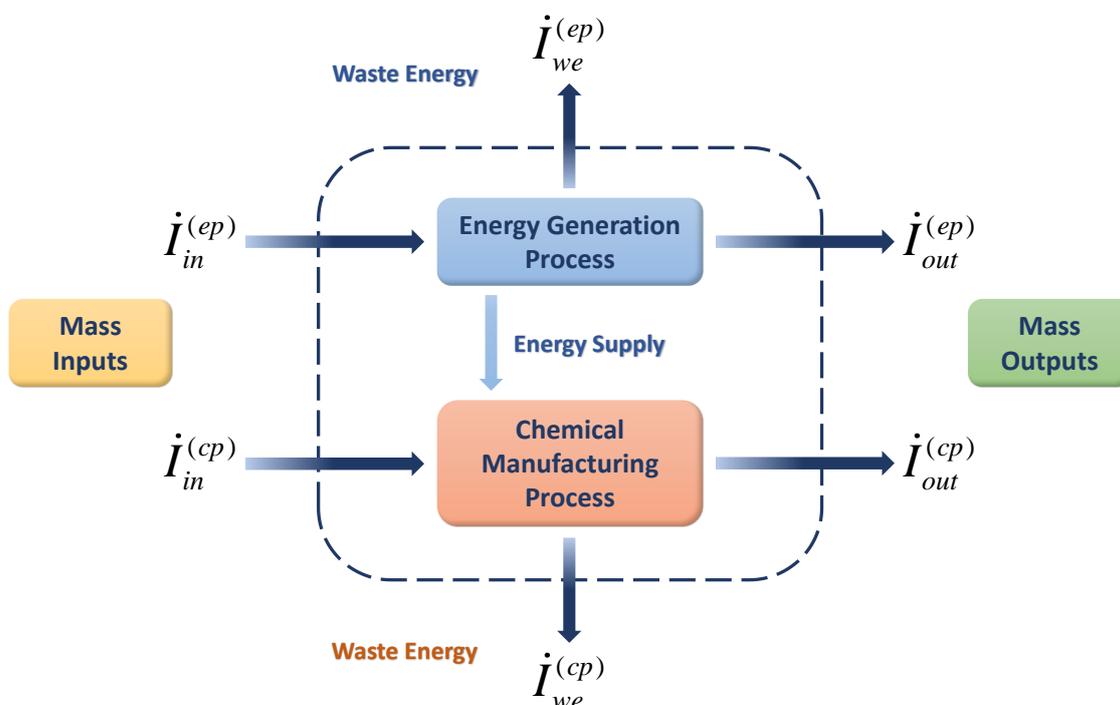


Figure 4: Boundary of PEI balance expression. Adapted from Young et al. (2000).

There are two classes of PEI indicators that can be derived from Equation (4): (i) the one associated with output, and (ii) the one associated with generation. As far as output indicators are concerned, this study uses the total rate of PEI output ($\dot{I}_{out}^{(tot)}$):

$$\dot{I}_{out}^{(tot)} = \dot{I}_{out}^{(cp)} + \dot{I}_{out}^{(ep)} \quad (5)$$

With regard to PEI generation, $\dot{I}_{gen}^{(syst)}$ may be a useful indicator of the internal environmental efficiency of a process (Young and Cabezas, 1999). In particular, it gives emphasis to the contribution of raw materials to the total PEI. For instance, output indicators do not capture the impact of switching from a non-renewable feedstock to a biomass derivative (Seay and Eden, 2009). However, we can anticipate that this is not the case of cumene manufacture, which is a well-established process based on benzene and propylene as raw materials (Degnan Jr et al., 2001). This consideration does not apply to energy generation as far as renewables are concerned. For now, being NG a major contributor to electric energy (EE) and steam generation, the relative importance of $\dot{I}_{in}^{(cp)}$ and $\dot{I}_{in}^{(ep)}$ will not be considered.

2.3 Multi-objective optimization

Once the indicators of economic and environmental sustainability are defined, it is possible to formulate the MOO problem. As reported by Azapagic (1999), the general MOO problem of a system takes on the following formulation:

$$\begin{aligned}
 \text{Min } \mathbf{f}(\mathbf{x}, \mathbf{y}) &= [f_1 f_2 \dots f_p] \\
 \text{s.t. } \mathbf{h}(\mathbf{x}, \mathbf{y}) &= \mathbf{0} \\
 \mathbf{g}(\mathbf{x}, \mathbf{y}) &\leq \mathbf{0} \\
 \mathbf{x} &\in \mathbf{X} \subseteq R^n \\
 \mathbf{y} &\in \mathbf{Y} \subseteq Z^q
 \end{aligned} \tag{6}$$

Where \mathbf{f} is a vector of economic and environmental objective functions to be simultaneously optimized, $\mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ and $\mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}$ are equality and inequality constraints, and \mathbf{x}, \mathbf{y} are the vectors of continuous and integer variables, which stand for material and energy flows, pressures, compositions, (discrete) sizes of process units, materials, and equipment. As discussed in Rangaiah and Bonilla-Petriciolet (2013), MOO problems do not feature a single solution that simultaneously optimizes conflicting objectives. Conversely, one is interested in determining the set of \mathbf{X} values that yield the best compromise solutions. These values are known as Pareto-optimal solutions, as the improvement of any one of the objectives is not possible without worsening at least one of other objectives. The MOO algorithm used in this paper is intentionally chosen amongst the brute-force methods, *i.e.* the grid-search method. This method can perform a robust and exhaustive evaluation of the objective function in the discretized domain of investigation provided that the number of degrees of freedom is reasonably low. The grid-search method, besides being exhaustive, can identify the absolute optima and allows drawing the hypersurfaces of the objective functions together with their contour lines. This allows gathering the optimality trends and the unique features of the MOO problem.

Another positive advantage of the grid-search method consists in the improved convergence of the process simulator that can rely on initial-condition values for a new simulation, which are inherited from the previous (*i.e.* adjacent) convergence point of the discretized grid. The results of plant simulations are k Pareto lines for each of the k price scenarios. The Pareto lines are only a two-dimensional projection of an n -dimensional hypersurface as in case of bi-objective optimization, which is the one involved in the assessment of economic and environmental sustainability. As none of the objective functions on the Pareto hypersurface can be improved without worsening the value of at least another objective function, some trade-offs among the objective functions are necessary in order to identify the preferred optimal solution based on a suitable decision criterion.

3 Case study

Cumene is one of the largest commodity derivatives of benzene, with an estimated production volume of 11.4 millions of tons in 2010. According to IEA (2013) this figure is expected to grow steadily in the next decades. Essentially, the whole cumene production is consumed for the synthesis of phenol and acetone. Eventually, phenol is used to produce both phenolic resins (to make furniture and construction boards) and polycarbonates, which have wide industrial applications (Shell, 2011). The synthesis of cumene involves (i) the reaction of benzene with propylene to form cumene, and (ii) the undesired reaction of cumene with propylene to form p-diisopropylbenzene (p-DIPB). Actually, the chemistry is more complicated due to the

formation of small amounts of heavier p-isopropylbenzenes (p-IPBs). However, for the sake of simplicity, this study accounts only for p-DIPB. A number of authors used the cumene process to illustrate plant-wide economic optimization (Luyben (2010); Gera et al. (2013); Norouzi and Fatemi (2012)), but few included environmental considerations (Sharma et al., 2013). At the best of our knowledge, nobody discussed the role played by market uncertainty on the size and operating conditions of plant equipment. Most studies drew inspiration from the basic flowsheet of Turton et al. (2008), where the byproduct is removed and used as fuel. However, conventional cumene plants convert p-DIPB back to cumene in a transalkylation reactor to reduce the loss of valuable product (Zhai et al., 2015). For this reason, we consider the process flow diagram of Pathak et al. (2011) that features the transalkylator of Figure 5. Pathak and coauthors provided a detailed description of the plant, thus this article recalls just the main aspects. For the sake of clarity, we chose to optimize a cumene production plant located in the USA.

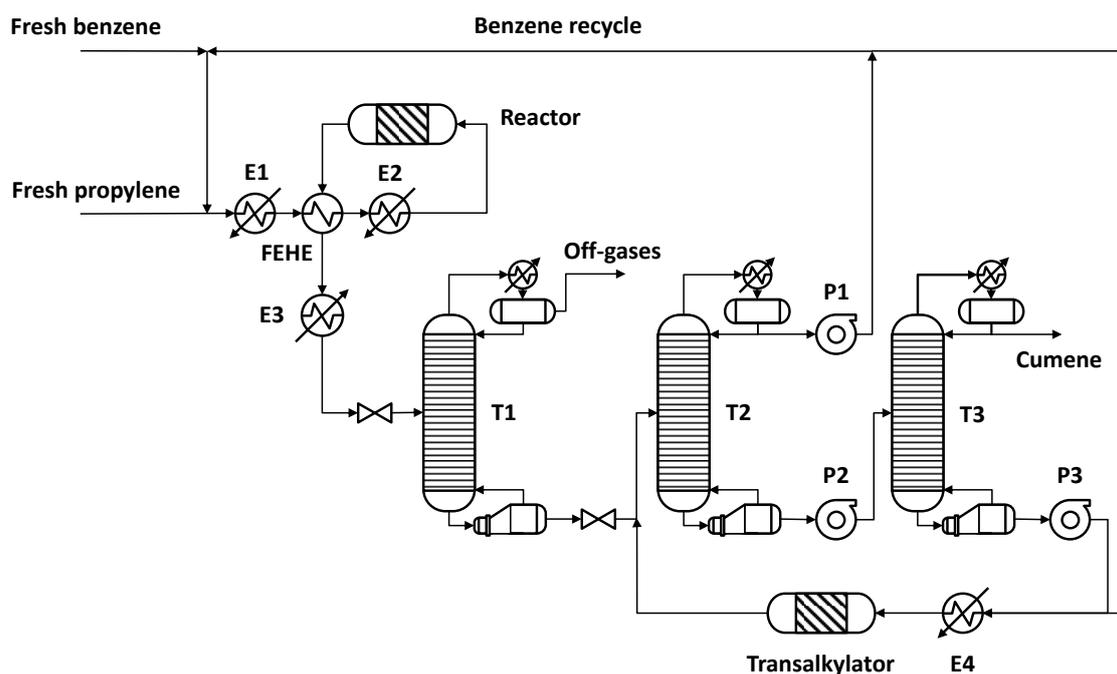


Figure 5: Cumene process flow diagram (adapted from Pathak et al. (2011)).

3.1 Process description

Table 1 reports the involved reactions and the corresponding kinetic schemes for the cumene synthesis. Selectivity is favored at low temperature, as the activation energy of the undesired reaction is higher than that of the synthesis reaction. In addition, selectivity improves by keeping the concentration of cumene and propylene low in the reactor, which requires a large excess of benzene that must be recycled.

Table 1: Chemical reactions and kinetic scheme of the cumene process (Pathak *et al.*, 2011). C_B : benzene concentration. C_P : propylene concentration. C_C : cumene concentration. x_B : benzene molar fraction. x_D : p-DIPB molar fraction. x_C : cumene molar fraction. R : 8.316 kJ/(kmol·K). Concentrations are in kmol/m³. Reaction rates are in kmol/(m³·s). For transalkylation, both forward ($r_{3,f}$) and reverse ($r_{3,r}$) reaction rates are reported.

Reaction	Kinetics
1 Cumene reaction $C_3H_6 + C_6H_6 \rightarrow C_9H_{12}$	$r_1 = 2.8 \cdot 10^7 \exp[-104,181 / (RT)] C_B C_P$
2 p-DIPB reaction $C_3H_6 + C_9H_{12} \rightarrow C_{12}H_{18}$	$r_2 = 2.32 \cdot 10^9 \exp[-146,774 / (RT)] C_C C_P$
3 Transalkylation $C_{12}H_{18} + C_6H_6 \rightleftharpoons 2C_9H_{12}$	$r_{3,f} = 2.529 \cdot 10^8 \exp[-100,000 / (RT)] x_B x_D$ $r_{3,r} = 3.877 \cdot 10^9 \exp[-127,240 / (RT)] x_C^2$

The plant designed by Pathak *et al.* (2011) has a nominal capacity of 95,094 t/y. The reactions occur in vapor phase in presence of a solid catalyst (assumed to have a solid density of 2000 kg/m³ and a void fraction of 0.5). Fresh benzene and fresh propylene enter the process as liquids at a rate of 98.96 kmol/h and 105.3 kmol/h, respectively. Fresh propylene contains 5% propane impurity, which is inert and has to be removed from the process. Since the separation of propylene and propane is difficult (Luyben, 2010), process economics favors high propylene conversion, which can be achieved by either increasing the reactor volume or operating at high temperature. The latter alternative increases the production of undesired byproducts, revealing the critical conflict between conversion (favored at high temperature) and selectivity (favored at low temperature).

As shown in Figure 5, fresh reactants are mixed with the benzene recycle, vaporized in E1, and preheated in two heat exchangers. The feed effluent heat exchanger recovers heat from the hot reactor outlet stream, while E2 heats the reactor inlet stream to the reaction temperature. The packed bed reactor recovers additional energy by generating high-pressure steam from the exothermic reactions. For the sake of completeness, Sharma *et al.* (2013) proposed an alternative heat integration system. However, the heat exchanger network synthesis is out of the scope of this paper.

The cooled reactor effluent is sent to a sequence of three distillation columns where the lightest component is separated first, according to the heuristics of Douglas (1988). Column T1 separates inert propane and any unreacted propylene (with a little benzene) as vapor distillate. The bottom from T1 is sent to column T2 that separates the unreacted benzene to be recycled. Finally, column T3 separates nearly pure cumene as distillate and p-DIPB as bottom. The p-DIPB stream is mixed with a fraction of the benzene recycle, heated, and fed to the transalkylator, whose effluent is sent to column T2 to recover benzene and cumene. Pathak *et al.* (2011) recommend adopting a heuristic approach to design the transalkylator, whose economic impact is limited as the inlet stream is relatively low (9.73 kmol/h in the base case). Pathak and coauthors set the inlet temperature at 240 °C (to avoid cumene dealkylation), the benzene to p-DIPB ratio at 2 (which provides good equilibrium conversion while controlling the benzene recycle), and the single-pass conversion at 75% (which is low enough to avoid an excessive increase of the reactor size). Thus, the smallest possible transalkylator has 100 packed tubes and is 1.6 m long.

The optimal design of the cumene plant offers some opportunities to reduce both the expenses and the environmental impact by (i) improving the performance and the selectivity, (ii) decreasing the formation of byproducts, and (iii) reducing the loss of raw materials and final products. According to Pathak *et al.* (2011), the most important design variables are the reactor inlet temperature, the reactor volume, the reactor pressure, and the benzene recycle fraction. The reactor inlet temperature affects both conversion and selectivity. In fact, higher temperatures increase the reaction rates and consequently the conversion. At the same time, higher temperatures decrease the selectivity, as the activation energy of the undesired reaction is higher than that of the synthesis reaction. In addition, higher temperatures result in greater energy costs.

The reactor volume has a relevant impact on the performance of the system. As the reactor volume increases, conversion improves, but a larger reactor is more expensive in terms of both vessel and catalyst cost. However, an increase in the reactor volume involves a decrease in the reactor inlet temperature and improves the selectivity. As far as the reactor pressure is concerned, it is worth operating at the maximum allowable pressure as the synthesis reaction occurs with a decrease in the number of moles. For this reason, the reactor pressure is fixed at 25 bar (Pathak et al. (2011)) and not optimized.

The recycle of benzene affects a number of important variables. For instance, when the recycle of benzene increases, the production of p-DIPB decreases, but the costs increase due to a larger recycle column. In summary, it is possible to reduce the synthesis of undesired byproducts by either decreasing the reactor inlet temperature or increasing the benzene recycle. For the sake of simplicity and robust flowsheet convergence, this study adopts as degrees of freedom of the MOO problem just the reactor inlet temperature and the reactor volume. This number of design variables is low if compared to other optimization problems in the literature (Gera et al. (2013); Norouzi and Fatemi (2012); Sharma et al. (2013)). However, this concern is not much relevant, as aim of this paper is not to carry out a sophisticated optimization, but rather illustrate an approach to the design of chemical plants for economic and environmental sustainability.

3.2 Economic sustainability

As anticipated in Section 3.1, the optimal plant configuration depends on two degrees of freedom: (i) reactor inlet temperature, and (ii) reactor volume. More specifically, being the number of tubes in the reactor fixed at 1500 (Pathak et al., 2011), the independent variable for reactor volume is assumed to be the tubes length. The upper and lower bounds for both the degrees of freedom are close to the ones proposed by Pathak et al. (2011), where the reactor inlet temperature does not exceed 390 °C to avoid hot-spot problems. Indeed, the reactor inlet temperature varies between 300 and 390 °C, and the reactor length between 4 and 10 m. The cumene plant is simulated at the steady-state condition with UniSim Design R430 (Honeywell, 2015), using the Peng-Robinson equation of state for the thermodynamic properties.

3.2.1 Conventional approach to the economic assessment of chemical plants

This Section discusses the conventional approach to the EA of chemical plants proposed in Douglas (1988). The utilities used in the cumene plant are the EE for pumps, the high-pressure steam in reboilers and heaters, and the cooling water in condensers and coolers. The conventional CD applied to the cumene plant presented by Pathak et al. (2011) entails the quantification of the fourth-level EP ($EP4$), defined as the difference between the revenues from selling the product and the CAPEX and OPEX terms associated with raw materials, reactors, separation system, and heat exchangers (Douglas (1988)). If the chosen time horizon is five years (Manca et al. (2011)), it is possible to address the sum of the $EP4$ over a corresponding period of sixty months:

$$\text{Cumulated } EP4 = \sum_{t=1}^{60} EP4_t = 60 \cdot EP4 \quad (7)$$

with $EP4$ in USD/mo and *Cumulated EP4* in USD.

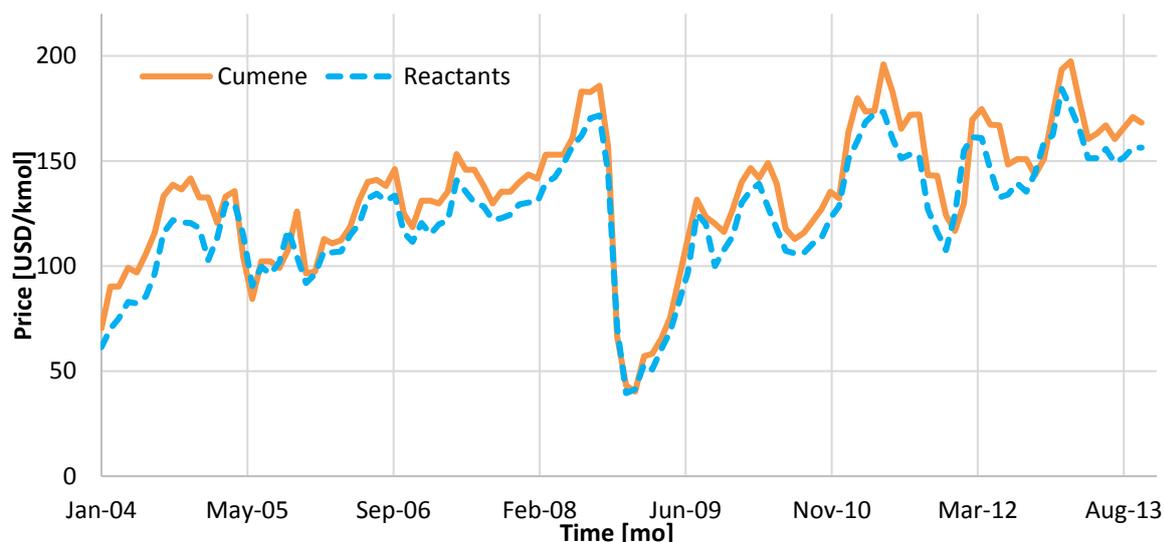


Figure 6: Comparison of monthly prices/costs of cumene and reactants from January 2004 to October 2013. Reactants cost was obtained by addition on mole basis. Equation (7) points to the last sixty months of the ten-year interval. It is worth pointing out that the historical quotations were considered only up to October 2013 due to the availability of information from databanks (e.g., EIA (2016b), ICIS (2016))

The CD approach of Douglas (1988) has a significant limitation that is epitomized by Equation (7). In fact, $EP4$ (see also Section 2.1 for further details) is supposed to be constant at every sampling time of the assessment period. Conversely, different values of $EP4$ can be calculated from each set of monthly quotations over the chosen time horizon. In fact, Figure 6 shows the volatility of cumene and reactants prices/costs in the 2004-2013 decade, which determines significant fluctuations of *Cumulated EP4* as summarized in Figure 7. Therefore, the conventional approach to EA is not representative of the economic sustainability of the cumene plant, because it suggests highly oscillating revenues (both positive and negative) that change according to the monthly prices/costs of both commodities and utilities.

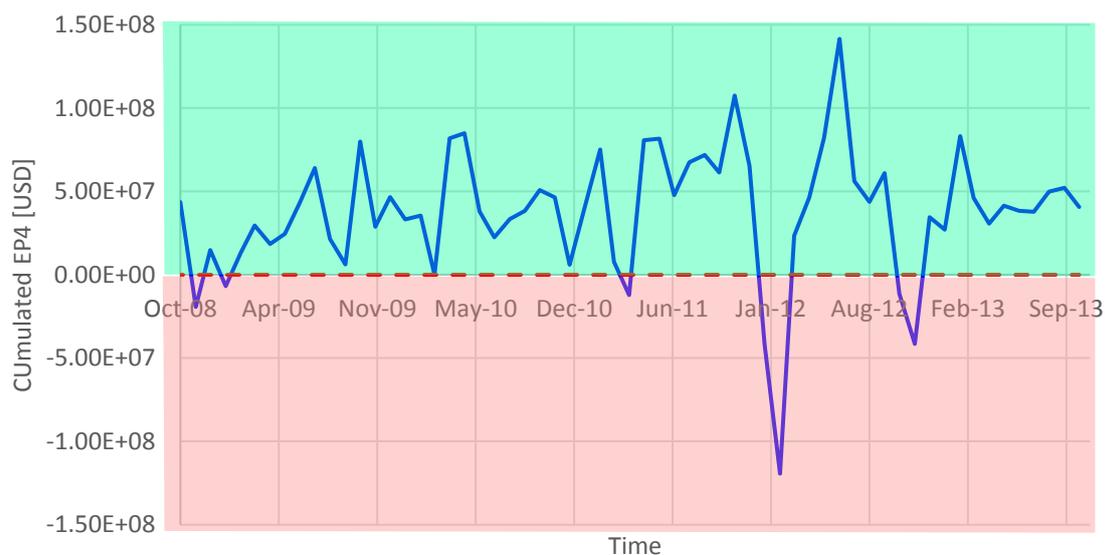


Figure 7: The EA based on the CD approach (i.e. fixed prices at a user-assigned specific time) would forecast either positive or negative EPs. The diagram displays the variable values of the *Cumulated EP4* as a function of the sixty monthly quotations from October 2008 to October 2013. The green area shows the profitable economic region; the red area shows the unprofitable one.

3.2.2 Economic assessment based on the PCD methodology

The EA according to PCD follows the steps shown in Figure 1 and Figure 2. CO is the precursor of each commodity involved in the cumene process, so it is chosen as the reference component. As already pointed out, we decided to optimize a cumene plant located in the USA, over an assessment period of five years (from October 2013 to October 2018) with monthly sampling as time granularity.

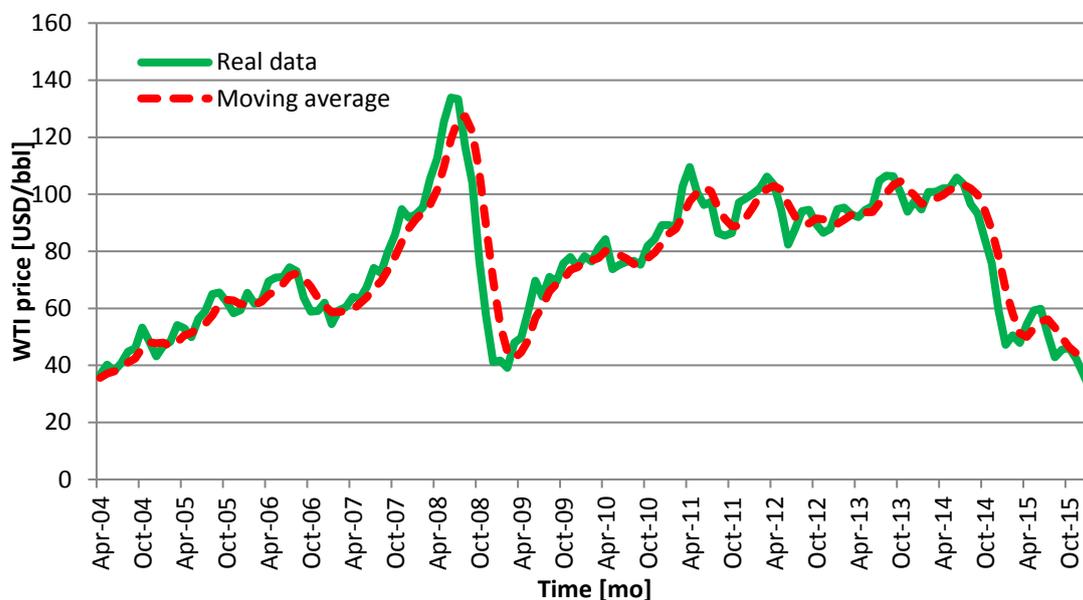
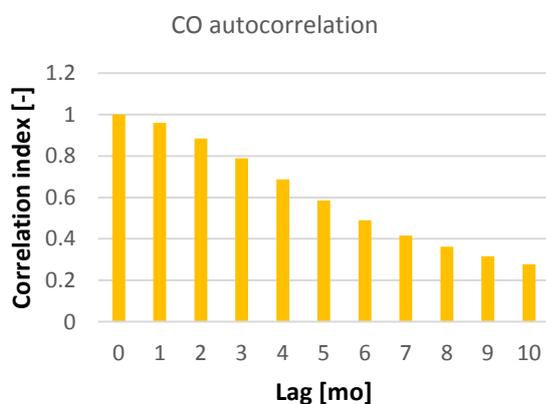


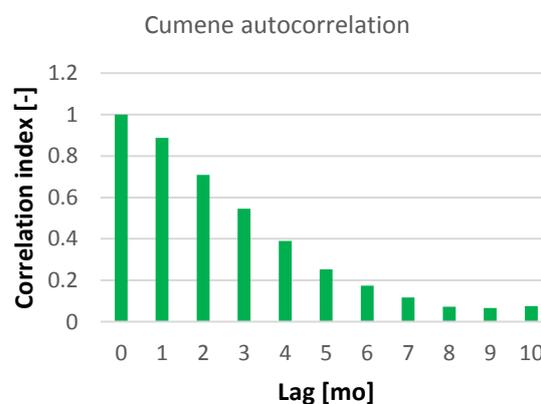
Figure 8: Comparison between historical WTI prices (green continuous line) and moving averaged prices (red dashed line) from April 2004 to January 2016 (monthly data from (EIA, 2016b)). The moving average is calculated over four quotations.

Figure 8 shows the historical time series of WTI prices (typical of the USA market instead of Brent quotations for the European market) and the comparison with the moving average prices. The usefulness of the moving-average operator is discussed in Barzaghi et al. (2016), and the EMs proposed here work with moving averaged quotations.

(a)



(b)



(c)

(d)

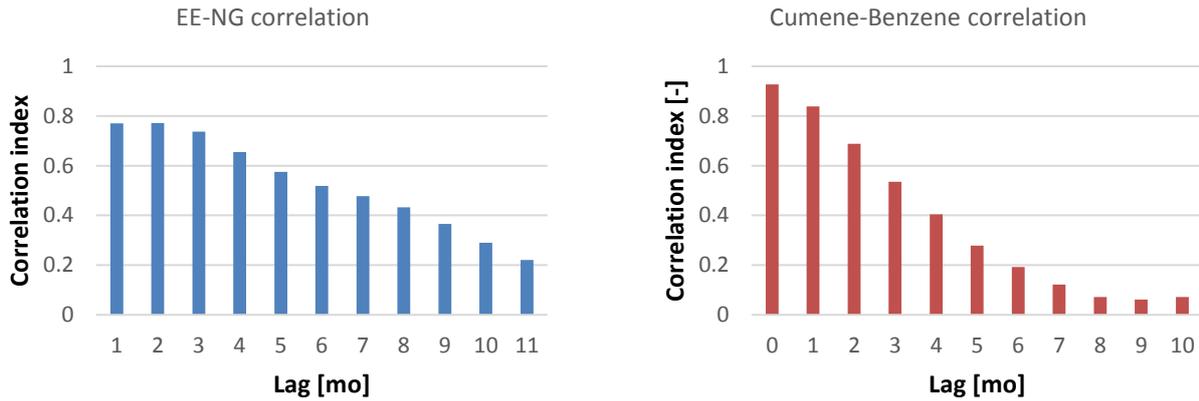


Figure 9: Autocorrelograms of CO quotations (a) and cumene prices (b), and correlograms of EE and NG prices (c), and cumene and benzene prices (d).

By analyzing the autocorrelogram shown in Figure 9a, one can deduce that the CO quotation at the i -th month depends mostly on two previous quotations. Therefore, the proposed EM of CO becomes (Manca, 2013):

$$P_{CO,i} = (A + B \cdot P_{CO,i-1} + C \cdot P_{CO,i-2}) \cdot (1 + rand \cdot \sigma_{CO} + \bar{P}_{CO}) \quad (8)$$

Where $P_{CO,i}$ is the i -th monthly quotation of WTI, σ_{CO} and \bar{P}_{CO} are the standard deviation and mean values of WTI price series, $rand$ is a stochastic function normally distributed, and A , B , and C are adaptive parameters that are calculated by a linear regression procedure that minimizes the mean square error between the real quotations and the model ones (Table 3).

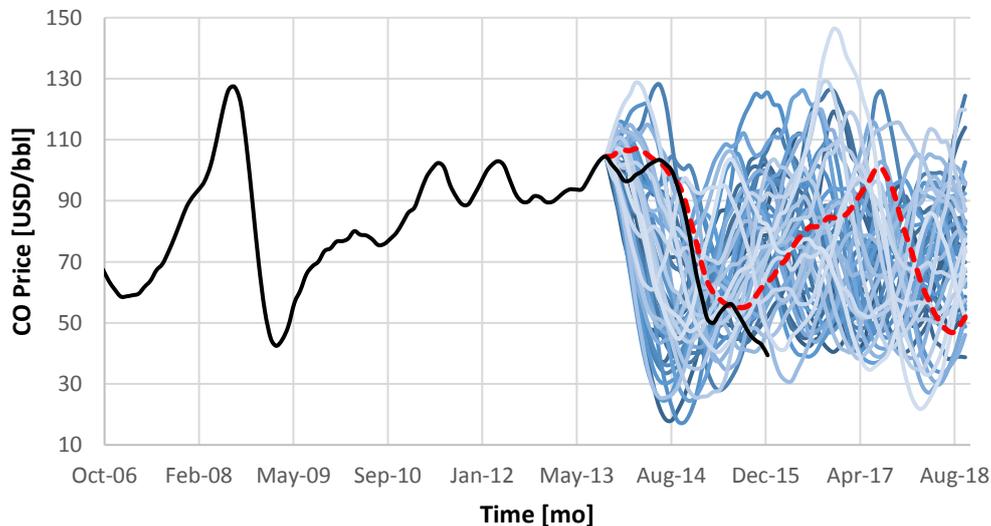


Figure 10: Chart of fifty possible CO future-price scenarios (cyan lines) over a five-year horizon from October 2013 to October 2018. The black continuous line shows the real CO prices up to November 2015 (EIA, 2016b). The red dashed line is the arbitrarily chosen scenario for the EA of the MOO problem.

Once identified, Equation (8) is used with a step-by-step approach to evaluate a distribution of future price scenarios (*i.e.* price trajectories), and obtain a probabilistic distribution of econometric scenarios (Figure 10).

For the sake of simplicity, the PCD procedure was carried out for just one arbitrarily chosen forecast scenario, *i.e.* the red dashed line of Figure 10 whose initial time is October 2013. This scenario is capable of

well forecasting the real WTI quotations from October 2013 to July 2015, while it departs from the real CO trend in the second half of 2015. Nonetheless, it can account for major oscillations. It is worth observing that the arbitrarily chosen scenario does not reproduce well the real quotations from July 2015 to January 2016 (*i.e.* the last real WTI quotation of this paper). This is primarily due to the abnormal events that affected the global economy (*e.g.*, Chinese crisis of stock exchanges, withdrawal of Iranian embargo, the USA overproduction of shale-oil, Saudi Arabia ruinous self-declared-leading position within OPEC, the Saudi Arabia vs Iran arm wrestling for oil quotas). In this regard, an economic approach to CO price modeling would be more flexible (Manca and Depetri, 2016), although more laborious and out of the scope of this article.

As far as the commodity EMs are concerned, we devised some tailored models for toluene, benzene, propylene, and cumene prices from a dedicated (auto)correlograms analysis as reported in Manca (2013). Indeed, Figure 9b and Figure 9d show the (auto)correlograms that were used to formulate the EM structure of cumene. Even though toluene is not directly involved in cumene manufacture, it is the precursor of benzene, and their prices are correlated. Table 2 lists the ADL models for the components of the cumene process, while Table 3 reports their adaptive coefficients.

Table 2 - ADL EMs for toluene, benzene, refinery grade propylene, and cumene prices.

Component	Model
Toluene	$P_{T,i} = A + B \cdot P_{CO,i} + C \cdot P_{CO,i-1} + D \cdot P_{T,i-1}$
Benzene	$P_{B,i} = A + B \cdot P_{T,i} + C \cdot P_{T,i-1} + D \cdot P_{B,i-1}$
Propylene (Refinery Grade)	$P_{P,i} = A + B \cdot P_{CO,i} + C \cdot P_{P,i-1} + D \cdot P_{P,i-2}$
Cumene	$P_{C,i} = A + B \cdot P_{B,i} + C \cdot P_{C,i-1} + D \cdot P_{C,i-2}$

The cumene process calls for the EA of a further (indirect) component, *i.e.* NG as it does not participate directly to the cumene synthesis but allows estimating the costs of most of the involved utilities, *i.e.* EE and steam (see also Table 4).

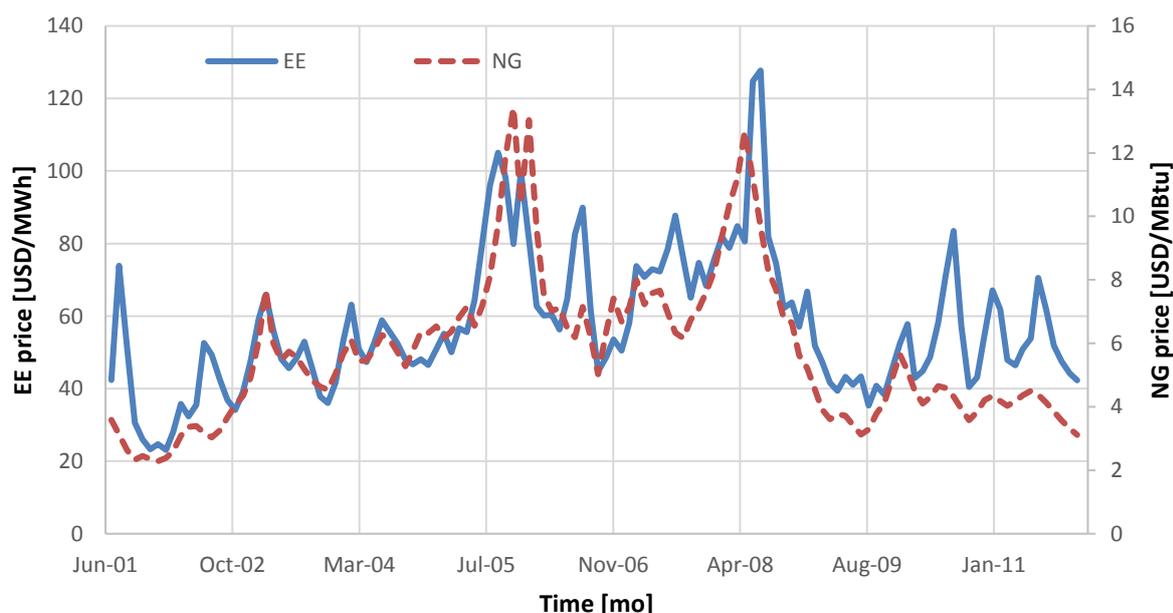


Figure 11: Comparison between EE prices and NG prices in the USA market from July 2001 to December 2011.

Indeed, Figure 11 highlights a significant dependency of the American EE prices from NG fluctuations. According to the correlogram analysis, NG quotations are correlated to the reference component with a time-delay of 8 months:

$$P_{NG,i} = (A + B \cdot P_{NG,i-1} + C \cdot P_{CO,i-8}) \cdot (1 + rand \cdot \sigma_{NG} + \bar{P}_{NG}) \quad (9)$$

Table 3 – Adaptive parameters of ADL EMs of CO, NG, toluene, benzene, refinery grade propylene, and cumene prices.

Raw material	A	B	C	D	R ²
Crude oil	3.128	0.966	-	-	0.951
Natural gas	0.914	1.091	0.0002	-	0.937
Toluene	1.331	0.767	-0.733	0.951	0.976
Benzene	-0.518	0.791	-0.726	0.943	0.969
Propylene (Refinery Grade)	2.737	0.084	1.588	-0.794	0.98
Cumene	10.993	0.487	1.287	-0.667	0.974

Respect to the rather complex modeling approach of Manca (2016) that was aimed at short-term horizon applications such as scheduling and planning, this paper focuses on a simpler ADL-derived approach based on the (auto)correlograms analysis and econometric dependency of EE from NG (Figure 9c) for long-term horizon applications such as PCD. Similar to EE, the steam price is assumed proportional to the NG quotations.

Table 4 - EMs for EE and steam prices.

Utility	Model
Electric energy	$P_{EE,i} = A + B \cdot P_{NG,i-1} + C \cdot P_{EE,i-1}$
Steam	$P_{STEAM,i} = A \cdot P_{NG,i}$

Table 5 - Adaptive parameters of EMs of EE and steam prices.

Utility	A	B	C	R ²
Electric energy	2.98	1.316	0.81	0.927
Steam	0.003	-	-	-

The multiplicative coefficient of steam model (Table 5) is obtained by assuming a fuel heat content of 1,029,000 Btu/Mcf (EIA, 2016a). In addition, the production of 1 klb/h of high-pressure steam (70 bar) requires a power of 1.2 MBtu/h that is provided by a proportional amount of NG fed to the boiler with 85% efficiency, which corresponds to 0.003 MBtu_{NG}/kg_{Steam} (DOE, 2016). In order to finalize the OPEX assessment, the cooling water cost and low-quality steam credits are those reported by Pathak et al. (2011), despite their negligible orders of magnitude respect to the other terms of the economic potential. Once the EMs are identified, it is viable to run the grid-search optimization to find the optimal set of degrees of freedom that maximize Equation (2) for the specific WTI scenario (sixty months) of Figure 10 (red dashed line). For the sake of clarity, the nominal capacity of 95,094 t/y (Pathak et al., 2011) is not kept constant during the optimization procedure, while the amounts of fresh benzene and propylene are fixed. Regarding the grid discretization, we chose a compromise between level of detail and computation load by assigning as discretization intervals 5 °C for inlet temperature, and 1 m for the tubes length. Consequently, the overall number of simulations over the discretized grid is 133. Since a few simulations at the boundaries

of the discretization domain were not successful (27%), only 97 simulations (based on the configurations of degrees of freedom) converged.

Figure 12 shows the contours of the *Cumulated DEP₄* surface as a function of the degrees of freedom. At the optimal solution, the inlet temperature is 365 °C and the reactor length is 7 m, while the *Cumulated DEP₄* is 10.15E6 USD. It is worth underling that the arbitrarily chosen WTI scenario (and all its derived EMs for both commodities and utilities) leads to five economically unsustainable solutions. For the sake of clarity, five grid points, with their corresponding coordinates, *i.e.* the degrees of freedom of the problem, are characterized by a negative *Cumulated DEP₄*.

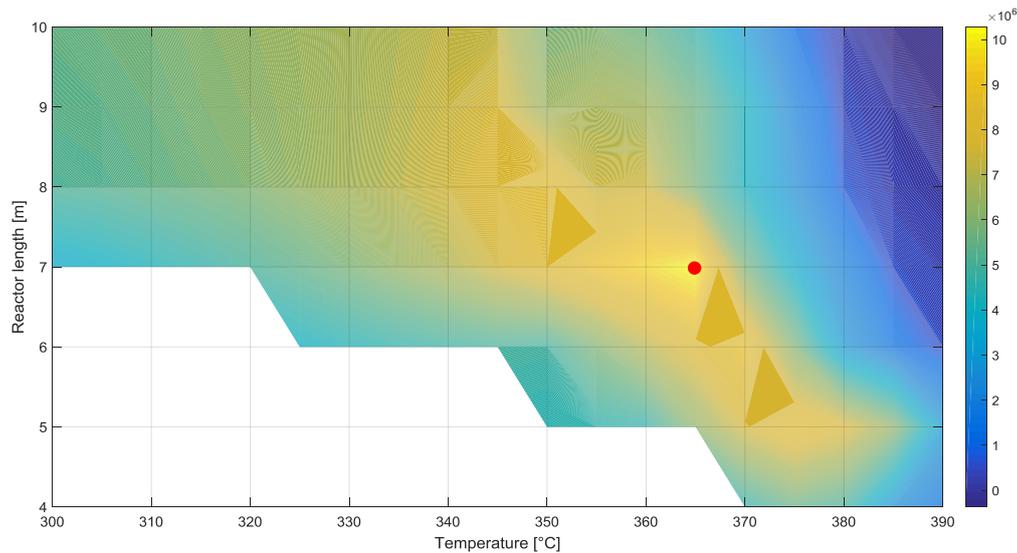


Figure 12: Contours of the Cumulated DEP₄ [USD] function with respect to inlet temperature and reactor length. The red point shows the optimal set of degrees of freedom for the EA based on the PCD method.

3.3 Environmental sustainability

According to the notation of Young and Cabezas (1999), the output PEI to the chemical process can be rewritten as:

$$\dot{I}_{out}^{(cp)} = \sum_j^{cp} \dot{M}_j^{(out)} \sum_k x_{kj} \psi_k \quad (10)$$

where $\dot{M}_j^{(out)}$ is the output mass flow rate of stream j , x_{kj} the mass fraction of chemical k in stream j , and ψ_k the overall PEI for chemical k . ψ_k can be calculated from:

$$\psi_k = \sum_l \alpha_l \psi_{kl}^s \quad (11)$$

where ψ_{kl}^s is the normalized specific PEI of chemical k for the impact category l , and α_l is the relative weighing factor of impact category l . The impact score of chemical k is normalized within each impact category to ensure that values from different categories contain the same units, and have on average equivalent scores (Young and Cabezas, 1999). The normalized impact scores are accessible from the WAR algorithm add-in included in the COCO Simulation Environment released by AmsterCHEM in collaboration with the USA EPA (Barrett et al., 2011). The weighing factors (α_l) express the relative importance of the impact categories (Table 6), and can range from 0 to 10 according to the specific concerns of the design engineer. This study assigns uniform weighing factors equal to unity, just to illustrate the general case where all the categories have the same importance.

Table 6: Environmental impact categories considered by the WAR algorithm (Barrett et al., 2011). The unit of LD₅₀ for human toxicity is the mass of chemical substance per body mass of target organism. OSHA PEL is the permissible exposure limit established for chemicals by the United States Occupational Safety and Health Administration. The unit of LC₅₀ for aquatic toxicity refers to fathead minnow, *i.e.* a small fish species.

General impact category	Impact category	Measure of impact category
Human toxicity	Ingestion	Lethal dose (50%) – LD ₅₀
	Inhalation/Dermal	OSHA PEL
Ecological toxicity	Aquatic toxicity	Fathead minnow LC ₅₀
	Terrestrial toxicity	LD ₅₀
Global atmospheric impacts	Global warming potential	GWP
	Ozone depletion potential	ODP
Regional atmospheric impacts	Acidification potential	AP
	Photochemical oxidation potential	PCOP

The normalized impact scores for all the chemicals used in this study are reported in Table 7. To provide a more exhaustive description of the impact across the battery limits of the plant, $\dot{I}_{out}^{(ep)}$ accounts for the reactants and product streams as fugitive emissions by means of a 0.001 multiplying factor (Smith et al., 2004), since chemical plants are likely to have relevant fugitive losses (Burgess and Brennan, 2001).

Similar to $\dot{I}_{out}^{(ep)}$, the output PEI of the energy generation process can be rewritten as:

$$\dot{I}_{out}^{(ep)} = \sum_j^{ep-g} \dot{M}_j^{(out)} \sum_k x_{kj} \psi_k \quad (12)$$

where the subscript *ep-g* refers to the gaseous output streams only, as the PEI of solid outputs can be assumed negligible compared to those of the gas outputs (Young and Cabezas, 1999). This study considers two conventional energy systems: a combined cycle gas turbine for the EE supply, and a large wall-fired boiler for the supply of steam to the chemical process.

Table 7: Normalized impact scores for the chemicals involved in the cumene process as provided by the WAR algorithm add-in included in the COCO Simulation Environment. The ODP is omitted since none of the chemical components contributes to that category. Values are in PEI/kg.

Chemical	HTPI	HTPE	TTP	ATP	GWP	PCOP	AP
Benzene	1.38E-01	2.26E-01	1.38E-01	1.06E-01	0	2.29E-01	0
Propylene	0	8.42E-03	0	0	0	3.83	0
Propane	0	4.02E-03	0	0	0	1.51E-01	0
Cumene	1.57E-01	2.96E-02	1.57E-01	4.11E-02	0	8.11E-01	0
p-DIPB	1.34E-01	0	1.34E-01	6.50	0	1.13	0
NO ₂	0	8.05E-01	0	0	0	1.57	1.08E-01
CO	0	1.32E-01	0	0	0	1.73E-01	0
CO ₂	0	8.05E-04	0	0	2.44E-04	0	0
SO ₂	0	5.57E-01	0	0	0	1.47E-01	1.54E-02
Methane	0	1.10E-02	0	0	5.61E-03	4.55E-01	0

Table 8 reports the pollutant emissions from both systems. NG used as fuel produces these emissions.

Table 8: Emission factors for the energy generation process (EPA, 2009). For the generation of electricity, a heat rate of 10408 Btu/kWh was assumed (EIA, 2016a). For the generation of steam, a fuel heat content of 1029000 Btu/Mcf was considered (EIA, 2016a), and the fuel energy per mass of steam was calculated as 1.2 MBtu/klb (DOE, 2016).

Chemical substance	Combined cycle gas turbine [lb/MBtu]	Large wall-fired boiler [lb/10 ⁶ scf]
NO ₂	0.32	190
CO	0.082	84
CO ₂	110	120000
SO ₂	0.0034	0.6
Methane	0.0086	2.3

Figure 13 shows the contour lines of the objective function and the optimal solution, *i.e.* the PEI minimum value. The optimal environmental solution (*i.e.* PEI equal to 3.417E6) is at an inlet temperature of 390 °C and a reactor length of 10 m, which corresponds to the very right upper bound of the discretized domain.

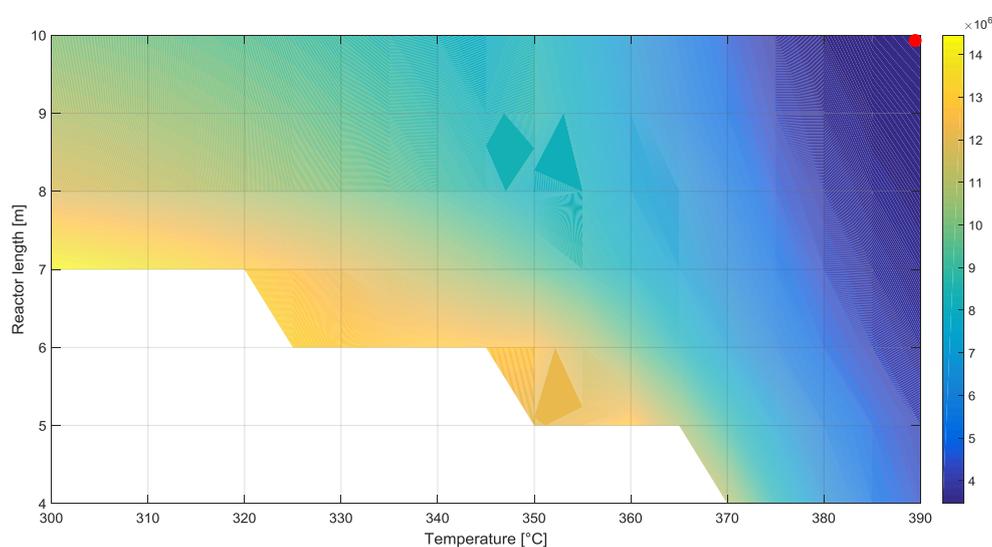


Figure 13: Contours of the PEI function with respect to inlet temperature and reactor length. The red point shows the optimal set of degrees of freedom.

3.4 Multi-objective optimization

Once both the economic and environmental objective functions are computed, it is possible to carry out the last step of Figure 1, *i.e.* the solution of the MOO problem and the selection of the best solution based on some trade-off between the different objectives. As already discussed in Sections 3.2 and 3.3, the elements of vector \mathbf{f} in Equation (6) are the objective functions *Cumulated DEP4* to be maximized (for economic sustainability) and $\dot{I}_{out}^{(tot)}$ to be minimized (for environmental sustainability). The functional dependency of both the economic and environmental performances is illustrated in Figure 14, which shows the Pareto curve generated by the arbitrarily chosen economic scenario of our MOO problem. The Pareto line features the so-called non-dominated solutions (*i.e.* configurations), where none of the objective functions can be improved without worsening the value of the others. Indeed, the plant configuration yielding the best economic performance (*i.e.* maximum of *Cumulated DEP4*) falls at the right end of the curve (point B of Figure 14) and corresponds to a temperature of 365 °C and a reactor length of 7 m. Conversely, the best environmental performance (*i.e.* minimum of $\dot{I}_{out}^{(tot)}$) falls at the left end of the Pareto line (point A of Figure 14) and corresponds to a reactor inlet temperature of 390 °C and a length of 10 m.

The Section 4 provides a discussion about the results and the best trade-off between the economic and environmental performances for the optimal design for sustainability of the cumene plant.

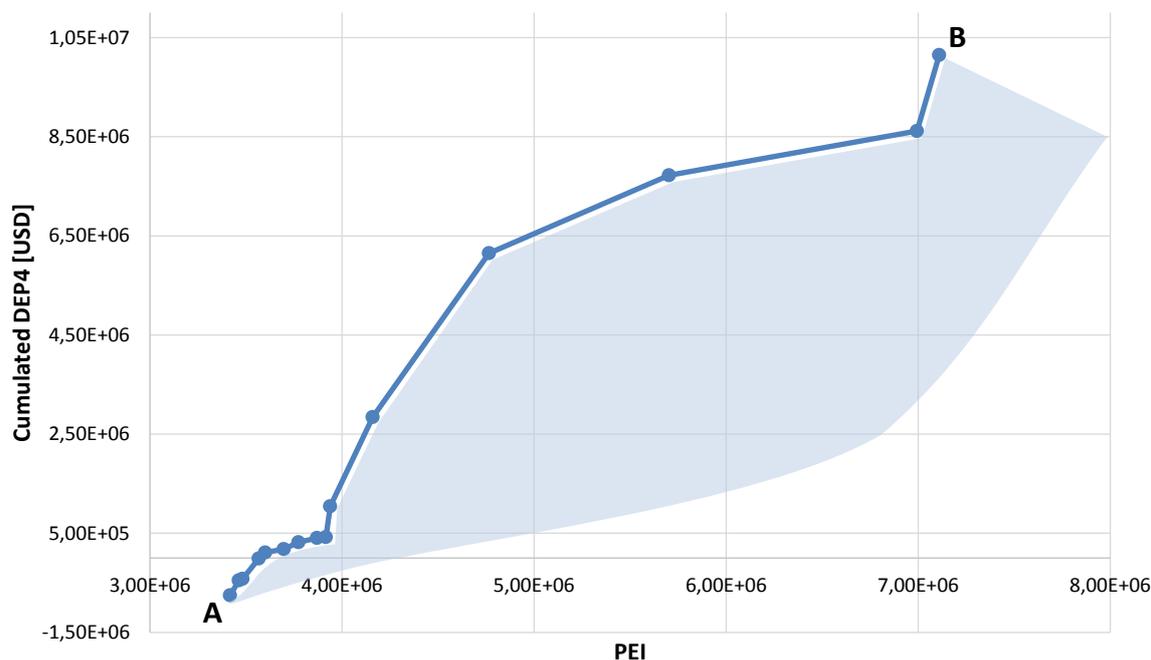


Figure 14: Pareto curve for the chosen economic scenario. The Pareto points correspond to the solutions of the MOO problem that are non-dominated (*Cumulated DEP4* better if higher; PEI better if lower).

4 Discussion of results

This Section is devoted to the assessment of the best trade-off between the maximum *Cumulated DEP4* and the minimum PEI. Based on the Pareto optimal solutions, the process engineer can choose among a number of alternatives depending on specific matters/criteria. Indeed, the configuration yielding the maximum *Cumulated DEP4* corresponds to a temperature of 365 °C and a reactor length of 7 m, while the minimum PEI is achieved at 390 °C and 10 m. As already discussed in Section 3.1, higher reactor inlet temperatures affect both conversion and selectivity, as an increase in conversion decreases the selectivity. In particular, higher temperatures contribute to the reduction of PEI as they increase the consumption of propylene, which has the highest total specific impact among the components involved in the process, apart from p-DIPB, whose emission is four orders of magnitude lower than that of propylene. At the same time, the decrease in selectivity plummets the *Cumulated DEP4* because of a reduced cumene production. As far as the CAPEX terms are concerned, shorter reactor lengths help enhancing the *Cumulated DEP4*, but both residence time and conversion get reduced. As a result, the economic optimum moves against the environmental best performance. In order to select a proper compromise, it is possible to identify the plant configuration that minimizes the geometrical distance from both the economic and environmental optima (Azapagic, 1999). According to this criterion, the candidate solution on the Pareto line corresponds to 385 °C and 5 m. It is worth observing that the environmental optimum corresponds to a higher temperature and a lower reactor length with respect to the economic maximum. Interestingly, the identified temperature trade-off is closer to the environmental optimum, while the corresponding reactor length is closer to the economic optimum. This may suggest that the environmental

performance is mainly affected by the decrease in selectivity because of propylene environmental impact, while the economic performance improves with a shorter reactor, *i.e.* by lowering the CAPEX terms.

5 Conclusions and future developments

Aim of the paper was to discuss a general methodology to reconcile environmental concerns with economic targets subject to market volatility and within the sustainability issue of chemical plants. The adopted methodologies were PCD for economic sustainability and WAR algorithm for environmental sustainability. Section 3.2 discussed how CD is unreliable when the economic sustainability of chemical plants under market uncertainty is concerned. Douglas' approach was outdone by PCD method with *Cumulated DEPA* being the optimal indicator for economic sustainability. PCD allows considering a probabilistic approach to future price scenarios and designing the cumene plant by looking at a suitable quotation scenario. On the contrary, the results of WAR algorithm and the corresponding PEI objective function do not depend on any economic scenarios.

As already remarked, the results presented in Section 3.4 and discussed in Section 4 refer to an arbitrarily chosen economic scenario, which is just one of the trajectories of future scenarios. It should be advisable to investigate the Pareto curve for a large number of scenarios and determine the statistical occurrence of a certain solution as the preferable MOO compromise. Future work will be devoted to illustrate in detail how to accomplish this task. Another limitation of this paper was considering a reduced number of degrees of freedom. Therefore, it would be worth increasing the number of decision variables according to the suggestions of Gera et al. (2013). Further developments will include the implementation of economic indexes that are more financially oriented and differ from Douglas' EPs, such as the net present value (NPV) and the internal rate of return (IRR). Eventually, future work will focus on the integration of social sustainability into a tri-objective decision-making problem.

Acknowledgments

The authors acknowledge the fruitful discussions on environmental sustainability and LCA with prof. Giovanni Dotelli.

Notation

ADL: Autoregressive Distributed Lag
AP: Acidification Potential
ARMAX: AutoRegressive Moving Average with eXogenous inputs
ARX: AutoRegressive model with eXogenous inputs
ATP: Aquatic Toxicity Potential
CAPE: Computer Aided Process Engineering
CAPEX: CAPital EXpenses
CD: Conceptual Design
CO: Crude Oil
COCO: CAPE-OPEN to CAPE-OPEN

DCD: Dynamic Conceptual Design
DEP: Dynamic Economic Potential
DOE: Department Of Energy
EA: Economic Assessment
EE: Electric Energy
EIA: Energy Information Administration
EM: Econometric Model
EP: Economic Potential
EPA: Environmental Protection Agency
FEHE: Feed Effluent Heat Exchanger
GWP: Global Warming Potential
HDA: HydroDeAlkylation
HTPE: Human Toxicity Potential by Exposure
HTPI: Human Toxicity Potential by Ingestion
ICIS: Independent Chemical Information Service
IEA: International Energy Agency
IRR: Internal Rate of Return
LC₅₀: Lethal Concentration to 50% of organisms
LCA: Life Cycle Assessment
LD₅₀: Lethal Dose to 50% of organisms
M&S: Marshall and Swift
MOO: Multi-Objective Optimization
NARMAX: Non-linear AutoRegressive Moving Average model with eXogeneous inputs
NARX: Non-linear AutoRegressive model with eXogeneous inputs
NG: Natural Gas
NPV: Net Present Value
ODP: Ozone Depletion Potential
OPEC: Organization of Petroleum Exporting Countries
OPEX: Operative Expenses
OSHA: Occupational Safety and Health Administration
PCOP: PhotoChemical Oxidation Potential
PDC: Predictive Conceptual Design
p-DIPB: para-diisopropylbenzene
PEI: Potential Environmental Impact
PEL: Permissible Exposure Limit
p-IPB: para-isopropylbenzene
PSE: Process Systems Engineering
TTP: Terrestrial Toxicity Potential
WAR: WAsTe Reduction
WCED: World Commission on Environment and Development
WTI: West Texas Intermediate

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