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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.

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 (CO_2) emissions to the atmosphere received great attention. Grossmann (2004) reported that the level of CO_2 in the atmosphere increased by a third since the beginning of the industrial age, and that CO_2 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

Abbreviations: 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; LC_{50}, Lethal Concentration to 50% of organisms; LCA, Life Cycle Assessment; LD_{50}, 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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the analysis of complex systems (Grossmann and Guillén-Gosálbez, 2010).Sustainability & Energy Systems

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 Fig. 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.

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