CHEMICAL ENGINEERING TRANSACTIONS
VOL. 43, 2015
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Chief Editors: Sauro Pierucci, Jiří J. Klemeš

ISBN 978-88-95608-34-1; **ISSN** 2283-9216
DOI: 10.3303/CET1543369

Economic Assessment of Chemical Plants Supported by Environmental and Social Sustainability

Piernico Sepiacci, Davide Manca*

PSE-Lab, CMIC Department, Politecnico di Milano, P.zza Leonardo da Vinci, 32 – 20133 Milan – Italy
davide.manca@polimi.it

Starting from the seminal definition of sustainable development (SD) proposed in 1987 by the World Commission on Environment and Development (WCED), this paper discusses how both environmental and social pillars of sustainability can be traced back to the economic one, which is the most important and consolidated amongst the three. The economic assessment of chemical plants goes through conventional methods of conceptual design. Manca (2013a) reported how raw materials, (by)products, and utilities, which as a whole contribute significantly to operative expenses (OPEX), are characterized by highly variable prices that call for a dynamic assessment of market quotations over a suitable time horizon. This manuscript shows how economic features such as market uncertainty, and price/cost volatility cannot be neglected whenever the economic sustainability of chemical plants is concerned. These issues are reconciled by an extended approach to conceptual design that takes into account the dynamic attribute, and allows identifying a set of possible economic scenarios based on forecasting the OPEX terms by means of suitable econometric or economic models.

1. Introduction

In 1979, the Engineers' Council for Professional Development defined engineering as “the profession in which a knowledge of the mathematical and natural sciences gained by study, experience, and practice is applied with judgment to develop ways to utilize, economically, the materials and forces of nature for the benefit of mankind” (CETS, 1986). According to Douglas (1988), chemical engineers contribute to the creation of new material wealth “via the chemical (or biological) transformation and/or separation of materials” by developing new processes, modifying, and optimizing existing plants. Process Systems Engineering (PSE) has traditionally been concerned with the understanding and development of systematic procedures for the design, control, and operation of chemical process systems (Sargent, 1991). Grossmann and Westerberg (2000) broadened the definition of PSE including “the discovery, design, manufacture, and distribution of chemical products in the context of many conflicting goals”. This definition relies on the concept of chemical Supply Chain (SC) as “a network of suppliers, production facilities, warehouses, and markets designed to acquire raw materials, manufacture, and store and distribute products among the markets” (Sahay and Ierapetritou, 2013). The wide-ranging approach of PSE to the physical, chemical, and biological processing operations covers a number of activities (e.g., conceptual design, data reconciliation, process optimization, planning and scheduling, SC management), and reflects the multi-objective nature of decision-making, whose variety of purposes is extremely broad.

The ongoing increase of social and environmental instances calls for implementing sustainability within the decision-making process in order to reconcile the economic goal with the social and environmental concerns. Sustainability is thought to be a wise balance among economic development, environmental conservation, and social equity (Sikdar, 2003). In 1987, WCED advocated a new era of economic growth where the needs of the present could be accomplished without compromising the ability of future generations to meet their own needs. This germinal definition of SD stands on the so-called three pillars of sustainability, i.e. economy, environment, and society. Sikdar (2003) identifies four types of sustainable systems: (i) systems referred to global concerns or problems, e.g., global warming, ozone depletion, use of genetically modified crops; (ii) systems characterized

Please cite this article as: Sepiacci P., Manca D., 2015, Economic assessment of chemical plants supported by environmental and social sustainability, Chemical Engineering Transactions, 43, 2209-2214 DOI: 10.3303/CET1543369

by geographical boundaries, e.g., cities, villages, defined ecosystems; (iii) systems based on businesses, either localized or distributed, which strive to be sustainable by practicing cleaner technologies, eliminating waste products and pollutant emissions, and reducing the energy intensity of processes; (iv) any particular technology that is designed to provide economic value through clean chemistries. Systems (iii) and (iv) are more suitable for the scope of chemical engineering as they depend more on process and product designs, and manufacturing methods.

To assess the sustainability of a system and more specifically of a chemical SC, there is need for measuring its performance. Despite the lack of a rigorous theory or definition, several sustainability measurement tools have been developed. For instance, IChemE presents three categories of indicators according to the pillars of sustainability. At the environmental level, IChemE classifies energy, material, water, and land uses. They propose as environmental impacts: acidification, global warming, human health, ozone depletion, photochemical smog formation, and ecological health. As economic indicators, IChemE identifies a number of value-added quantities, and the R&D costs. Finally, the social indicators are based on employee benefits, safety, and how employees are treated by the company. As a further example, Azapagic and Perdan (2000) proposed an interconnected structure of indicators based on those three pillars. Economic indicators comprise financial and human-capital subsections. The human-capital indicators are employment contribution, staff turnover, expenditure on health and safety, and investment on staff development. Social indicators address ethics and welfare. As far as welfare indicators are concerned, the authors classify income distribution, work satisfaction, and accomplishment of social needs. According to this framework, each sustainability pillar has a distinct identity but at the same time contains influences from the other pillars. For instance, the human-capital subsection of the economic indicators is rooted in the social pillar. Something similar happens to the welfare subsection of the social indicators that depends rather on the economic performance. The environmental indicators are even more related to the economic pillar. Indeed, Azapagic and Perdan (2000) observed that environmental indicators often refer to material and energy consumptions that can be easily converted into economic quantities. For instance, the chemical industry often employs as environmental indicators: energy consumed, waste production, and by-products recycling. These indicators can be normalized to a single measure by means of suitable metrics based on economic criteria.

This illustration suggests that both the environmental and social aspects of sustainability can be traced back to the economic one as far as the feasibility of industrial processes is concerned. This point leads the way for the discussion of chemical products and processes under the perspective of economic sustainability. Despite its relevance, the economic pillar is probably the most elusive amongst the three. However, it requires being specifically assessed. When referring to economic sustainability, some authors draw attention to the risk associated with market fluctuations (Carter and Rogers, 2008), and observe that traditional economic performance measures neglect the dynamic attribute of prices and costs over time (Bakshi et al., 2003). This paper discusses the uncertainties that affect the long-term profitability of chemical plants (e.g., market volatility, price/cost oscillations), and presents a methodology based on suitable econometric models to improve the reliability of feasibility studies.

2. Economic sustainability

In light of the recent trend on developing more sustainable technologies, PSE has intensified its efforts in providing advanced tools for the design, optimization, and retrofitting of chemical processes. The biggest challenge is to reconcile a number of independent and often conflicting objectives, which must be considered simultaneously. The focus is frequently on the relation between economic and environmental performance, so that operational and environmental targets are combined by means of suitable trade-offs. According to Grossmann and Guillén-Gosálbez (2010), many of the existing methods, adopted in both process synthesis and SC management, fail to account for the sources of uncertainty that may occur in practice (e.g., volatility of prices/costs, market fluctuations, offer/demand oscillation, climate change, seasonal/annual periodic variations, natural disasters). Traditionally, the uncertain parameters are assigned with a nominal value, thus their variability is neglected. This simplification may lead to solutions that perform well in most scenarios but lose reliability under unexpected conditions. As an example, Ouattara et al. (2012) revisited the process for the hydrodealkylation (HDA) of toluene to produce benzene under an economic and environmental approach. They formulated a multiobjective nonlinear optimization problem in order to maximize the benzene production, and minimize both the annual cost and the environmental impact. As usual, the evaluation procedure of OPEX assumes constant the prices/costs of raw materials, products, and utilities. This is a significant limitation whenever one performs an economic assessment 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 mutually oscillate below and over one another thus making the plant production either fruitful or fruitless as a function of market quotations (Manca, 2013a). Figure 1 shows for the HDA process the continuously crossing trends of benzene price (i.e. product) and toluene cost (i.e. raw material) over a long-term horizon. In the time intervals when the price of benzene is lower than the cost of toluene, the necessary condition for the economic sustainability of the process is not met and the HDA plant should not be operated.

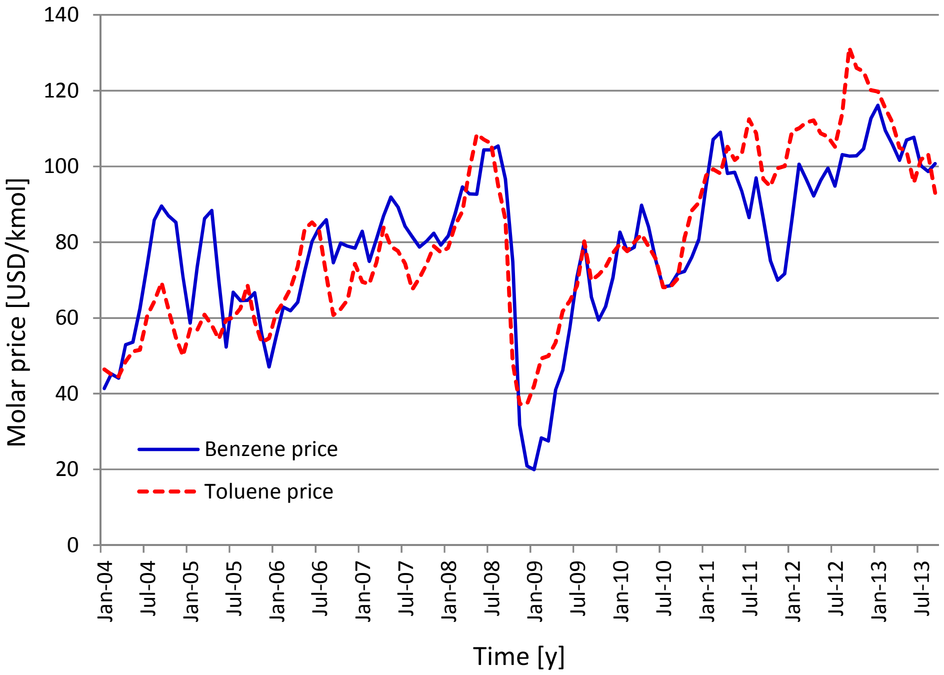

Figure 1: Monthly quotations of toluene and benzene over a long-term horizon.

Manca and coworkers (Manca, 2013a; Rasello and Manca, 2014) reported a number of cases where raw materials, commodities, and utilities witnessed high variations of prices in short- and medium-term periods. For instance, the trend of crude oil (CO) quotations can be observed as a paradigmatic example of how commodities may fluctuate with big oscillations. Actually, CO is a suitable representative of several derivatives in the process industry. In the first months of 2007, CO was quoted at about 50 USD/bbl, and its price continued to increase steadily for almost 16 months until the end of the second quarter of 2008, when it reached the highest ever value at 140 USD/bbl. Next, the US subprime crisis of 2008 triggered a very tough recession period for most countries. In the second semester of 2008, the CO price witnessed a four-fold contraction touching a minimum of 35 USD/bbl. The repercussions were both financial and industrial.

Most commodities that are derived from CO as either direct distillates (e.g., gasoil, diesel, naphtha, kerosene, burning oil) or petrochemical derivatives (e.g., natural gas, petroleum gas, coal) see their prices tightly bound to those of raw materials used for their production. Similar remarks can be drawn for utilities such as electric energy, which not only suffer from both financial and economic causes, but are also dependent on national markets, and get influenced by weather conditions, strikes, embargos, and political and investment decisions. In the light of the dynamic characteristic of OPEX terms, next Section presents a methodology based on econometric models to assess the economic sustainability of chemical plants. For the sake of brevity, further discussions on the environmental and social contributions are not reported. However, it is suggested to implement the following methodology even when both environmental and social sustainability are concerned.

2.1 Dynamic conceptual design

Feasibility studies of chemical plants are based on assessing both CAPEX (i.e. capital expenses) and OPEX terms. When it comes to OPEX assessment the prices and costs of raw materials, (by)products, and utilities are assumed constant; their value being usually referred to the time when the study is performed. As already remarked, this approach can be highly risky as the dynamic fluctuations of markets and prices/costs variability are completely neglected. Therefore, it is advisable to change approach and implement quantitatively the dynamic attribute. Instead of assuming fixed the prices/costs over long-time periods, as in the conventional and widely adopted approach of Douglas (1988) to conceptual design, it is recommended to determine a class of dynamic models of prices/costs so to forecast the market volatility over the rather long-time horizon of feasibility studies. Technically speaking these models can feature either an econometric or an economic approach to modeling, which is respectively based on either identifying a functional relationship between dependent and independent variables or grounding the mathematical relationship on market variables that play a direct role on those fluctuations.

Manca (2012, 2013a) discussed how to structure and identify an econometric model (EM) by implementing the following actions: (i) identification of a reference component; (ii) identification of the sampling time and time horizon; (iii) identification of an EM of the reference component: (iv) EMs identification of the raw material(s), byproduct(s), and product(s); (v) EMs identification of the utilities; (vi) use of the identified EMs to assess dynamically the economic impact of the chemical plant under design.

The idea behind action (i) is that it would be advisable to identify a reference component whose economic role is conditioning the quotations of other derived products. As far as commodities are concerned, most of them are derived, extracted, and produced by treating, distilling, and separating fractions of CO. For this reason, CO is a good candidate for the econometric models as it plays the role of independent variable. By identifying a reference component, the quotations of derivatives can be parameterized and referred to its dynamic trend. Both econometric and economic models are time-discrete. Therefore, they allow evaluating future trends according to a suitable sampling time whose value is a function of the time horizon of the feasibility study (see action (ii)). As that study covers quite a number of years (according to the conceptual design approach) the sampling time is usually assumed to be either one month or one quarter. Action (iii) identifies the econometric/economic model of the reference component. This action consists of determining the adaptive parameters of the model by studying the behavior of historical trends of CO quotations. This model comprises both deterministic and stochastic values. Role of the stochastic values is to depict the plethora of possible future scenarios so to describe stable/bullish/bearish trends and find a distribution of expected/reasonable circumstances based on historical values. Rasello and Manca (2014) proposed the following model of CO quotations based on the hypothesis of Markovian process:

$$P_{CO,i} = P_{CO,i-1}\left(1 + RANDN \cdot \sigma_{CO} + \overline{X}_{CO}\right) \quad (1)$$

where $P_{CO,i}$ is the price of CO at $i-th$ time interval, $\sigma, \overline{X}$ are the standard deviation and average value of the historical trend and $RANDN$ is a function that produces a random normal distribution. Action (iv) consists of identifying the econometric models for all the components present in the process/plant under design. A nonlinear regression routine evaluates the adaptive parameters of these models by minimizing the distance between the model values and the real prices/costs. Action (v) works with the same approach adopted in action (iv) but focuses on utilities such as steam, fuel oil, and electric energy (Manca, 2013b).

Once the ingredients necessary to the dynamic assessment of the feasibility study are available (i.e. actions (i-v)), it is time to use a specific procedure to quantify the OPEX terms over the time horizon of the conceptual design. The proposed approach consists in expanding the hierarchical method of Douglas (1988), which is based on constant price/cost values, to a dynamic assessment that considers different scenarios with prices and costs subject to markets volatility. The fan of scenarios is covered by the stochastic contribution reported in Eq. (1) and is quantified by suitable economic potentials featuring the aforementioned dynamic attribute. Eq. (2) describes how $DEP4$, i.e. the dynamic economic potential of fourth level (in line with Douglas' static counterpart, $EP4$), is formed. The resulting feasibility study is framed within the Dynamic Conceptual Design (DCD) methodology, as discussed in Manca and Grana (2010).

$$Revenues4_{i,k}\left[\$/h\right] = \max\left[0, \left\{\sum_{p=1}^{NP} C_{p,i,k} \cdot F_p - \sum_{r=1}^{NR} C_{r,i,k} \cdot F_r - \sum C_{EE,i,k} \cdot W_{electr} - \sum C_S \cdot F_S - \sum C_{H_2O} \cdot F_{H_2O} - C_{FO,i,k} \cdot F_{FO}\right\}\right] \quad (2)$$

$$DEP4_k\left[\$/y\right] = \frac{\sum_{i=1}^{nMonths}\left(Revenues4_{i,k} \cdot nHpM\right)}{nMonths/12} - \frac{\sum_{e=1}^{nEquip}\left(IC_e\right)}{nMonths/12} \qquad k = 1, \ldots, nScenarios$$

Where N_P, N_R are the number of (by)products and raw materials; C, F are the price/cost of process streams and their corresponding flowrates; $nHpM$,$nEquip$ are the number of production hours in a month, and the number of process units involved in the economic assessment; W, IC are the electric power absorbed by a specific unit, and the investment cost of equipment; S, H_2O, FO are the subscripts that identify respectively the steam used in the reboilers of the distillation columns, the water used in the condensers of those columns, and the fuel oil used in the furnace of the plant. Eq. (2) considers both CAPEX and OPEX terms. The $\max$ function translates mathematically the concept that the plant should run only when the revenues are positive, i.e. when the incomes are higher than the expenditures for each $i-th$ discretization time. Index k transforms the classical conceptual design from a deterministic assessment (based on one $EP4$ value) to a stochastic one, which is characterized by a distribution of possible future trends of the $DEP4_k$ terms.

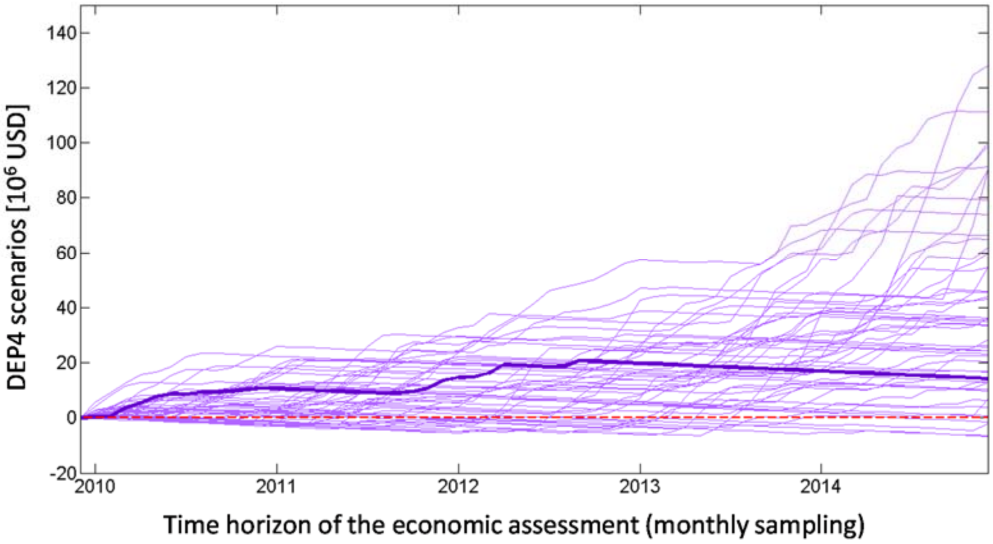

Figure 2: Probabilistic distribution of DEP4 cumulative profiles for a set of fifty different economic scenarios applied to a chemical plant over a five-year horizon. The bold line highlights just one of the simulated scenarios.

For the sake of clarity, the cornerstone of the DCD methodology is symbolized by the $nScenarios$ parameter, which requires that a set of different scenarios are evaluated according to the price/cost trajectories obtained by the aforementioned EMs through their constitutive stochastic contributions. Therefore, k subscript of each $DEP4$ takes to a probabilistic concept of DCD that is founded on the distribution of possible economic scenarios of the plant. Figure 2 shows a number of different scenarios based on the trajectories that the cumulative $DEP4$ of Eq. (2) would assume over a 5-year forecasting horizon (i.e. 2010-2014) according to the stochastic fluctuations of prices/costs of raw materials, (by)products, and utilities as described by the EMs discussed above.

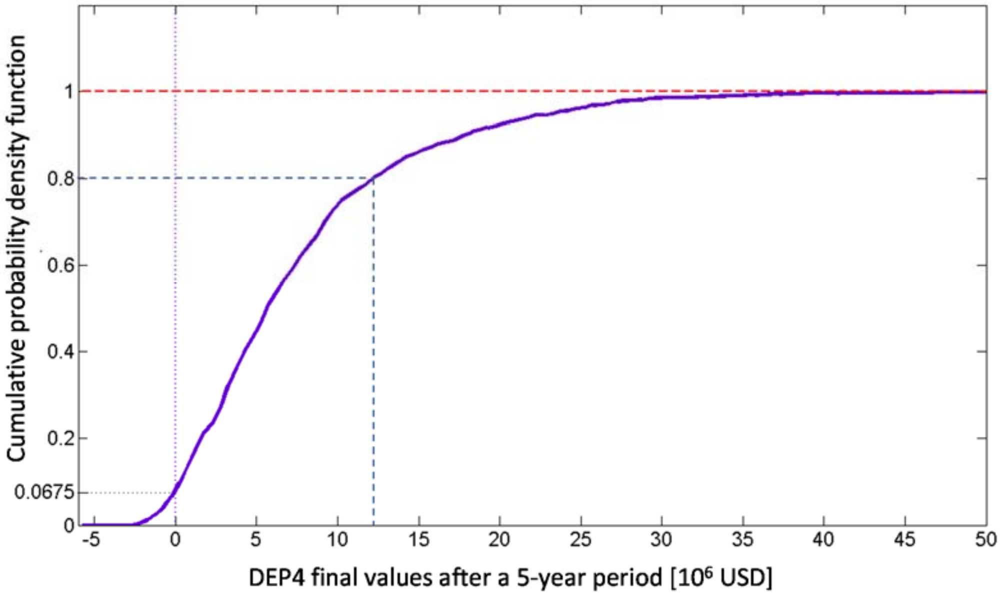

Figure 3: Cumulative density function of the dynamic economic potentials of fourth level, DEP4.

To better understand and summarize the distribution of economic scenarios, Figure 3 shows the cumulative density function of possible $DEP4$ values after a 5-year forecasting period. The curve is obtained from a wide range of different economic scenarios (i.e. 5,000) and shows, for instance, that there is a probability of 6.75% that after five years the economic potential of fourth level is still negative. In addition, 80% of the possible scenarios forecast a fourth-level economic potential after five years that is below $12 million. Figure 3 calls for a mindset change based on accepting that uncertainty plays a primary role on future quotations, and that demand oscillation and market volatility may significantly affect the economic sustainability in terms of operation of plants and profitability of processes.

3. Conclusions

The paper suggested how the environmental and social pillars of chemical plants sustainability can be taken back to the economic one, and how conceptual design of chemical plants can obtain a significant improvement in reliability by implementing econometric models based on stochastic elements for the dynamic assessment of the feasibility study. Similar approaches can also be adopted to evaluate the sustainability of products and SCs. The paper discussed and showed how it is advisable to use the $DEP4$ in place of the traditional economic indicators (e.g., profit-potential, annual cost, NPV, DCFRR) adopted in most sustainability studies (Othman et al., 2010; Ouattara et al., 2012; Zheng et al., 2012; Yue and You, 2013).

References

Azapagic A., Perdan S., 2000, Indicators of sustainable development for industry: A general framework, Process Safety and Environmental Protection, 78(4), 243-261.

Bakshi B. R., Fiksel J., 2003, The quest for sustainability: Challenges for process systems engineering, AIChE Journal, 49(6), 1350-1358.

Carter C. R., Rogers D. S., 2008, A framework of sustainable supply chain management: Moving toward new theory, International Journal of Physical Distribution and Logistics Management, 38(5), 360-387.

CETS, 1986, Engineering infrastructure diagramming and modeling, Engineering Education and Practice in the United States, National Academy Press, Washington, DC, USA.

Douglas J. M., 1988, Conceptual Design of Chemical Processes. McGraw-Hill, New York.

Grossmann I. E., Guillén-Gosálbez G., 2010, Scope for the application of mathematical programming techniques in the synthesis and planning of sustainable processes, Computers and Chemical Engineering, 34(9), 1365-1376.

Grossmann I. E., Westerberg A.W., 2000, Research challenges in process systems engineering, AIChE J., 46, 1700-1703.

Manca D., 2012, A Methodology to Forecast the Price of Commodities. Computer Aided Chemical Engineering, 31, 1306-1310.

Manca D., 2013a, Modeling the commodity fluctuations of OPEX terms, Computers and Chemical Engineering, 57, 3-9.

Manca D., 2013b, A methodology to forecast the price of electric energy, Computer Aided Chemical Engineering, 32, 679-684.

Manca D., Grana R., 2010, Dynamic Conceptual Design of Industrial Processes. Computers and Chemical Engineering, 34, 656-667.

Ouattara A., Pibouleau L., Azzaro-Pantel C., Domenech S., Baudet P., Yao B., 2012, Economic and environmental strategies for process design, Computers and Chemical Engineering, 36(1), 174-188.

Othman M. R., Repke J., Wozny G., Huang Y., 2010, A modular approach to sustainability assessment and decision support in chemical process design, Industrial and Engineering Chemistry Research, 49(17), 7870-7881.

Rasello R., Manca D., 2014, Stochastic price/cost models for supply chain management of refineries. Computer Aided Chemical Engineering, 33, 433-438.

Sahay N., Ierapetritou M., 2013, Supply chain management using an optimization driven simulation approach. AIChE Journal, 59(12), 4612-4626.

Sargent R.W.H., 1991, What is chemical engineering? CAST Newsletter, 14(1), 9-11.

Sikdar S.K., 2003, Sustainable development and sustainability metrics, AIChE Journal, 49(8), 1928-1932.

WCED, 1987, Our Common Future. Oxford University Press.

Yue D., You F., 2013, Sustainable scheduling of batch processes under economic and environmental criteria with MINLP models and algorithms, Computers and Chemical Engineering, 54, 44-59.

Zheng K., Lou H. H., Gangadharan P., Kanchi K., 2012, Incorporating sustainability into the conceptual design of chemical process-reaction routes selection, Industrial and Engineering Chemistry Research, 51(27), 9300-9309.