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Process Design With Dynamic Superstructures

Davide Manca and Roberto Grana
CMIC Department "Giulio Natta", Politecnico di Milano
Piazza Leonardo da Vinci, 32, 20133, Milano, ITALY, davide.manca@polimi.it

This paper focuses on chemical process design and layout optimization based on a novel approach. As originally conceived, conceptual design and systematic process design assume both prices and costs as fixed. Conceptual design does not account for well-known price fluctuations such as electric energy price and raw material costs. This classic approach to process design may find a sub optimal solution since it neglects the economic dynamic changes occurring in a defined time horizon. This manuscript modifies the viewpoint and considers the daily fluctuations of electric energy price inside the conceptual design activity, in order to maximize the so-called economic potential. A straightforward case study, based on an energy intensive chemical process, shows the benefits and the opportunities of this approach. The mathematical model is based on the implementation of dynamic superstructures that call for a MINLP formulation. Finally, the manuscript presents and discusses some numerical results.

1. Introduction

The optimal design of chemical and industrial processes is a complex problem that involves several facets. Nowadays, some of them are well understood and fully implemented, whereas others are still not and they deserve further attention as open issues in both scientific and industrial communities. Some papers in the scientific literature (*e.g.* Cruse *et al.* (2000); Iršič Bedenik *et al.* (2007)) focused on the integration of conceptual design, market uncertainties, and dynamic optimization. Specifically, this manuscript discusses the process design optimization, in terms of conceptual design. The term conceptual design deals with an optimization problem where specific superstructures are selected according to some criteria (Biegler *et al.*, 1997). A superstructure summarizes a few process alternatives that are selected by corresponding sets of Boolean/integer variables. The conceptual design procedure cuts off the suboptimal equipment layouts while identifying the best one according to economical, environmental, and safety criteria. Often, the resulting problem is a multi-objective optimization where continuous variables and geometric specifications are mixed with integer and Boolean decision variables. The classic conceptual design is a steady-state problem, based on fixed costs and prices. Conversely, this paper focuses on the dynamic evolution of markets (*e.g.* electric energy price, utility and raw material prices). By doing so, the process layout derived by the steady state approach to conventional conceptual design can strongly differ from the solution of a dynamic conceptual design.

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2. Price Fluctuations and Dynamic Superstructures

Raw materials, products, utilities, and equipment are subject to significant price/cost oscillations often due to unexpected and difficult to predict economic factors (Bonfill *et al.* (2004)). Chemical process design can account for these fluctuations, which are quoted in the market, in order to increase the detail and reliability of the so-called economic potential (according to Douglas' terminology, 1988). For instance, the electric energy price has a well-known daily quotation: in fact, during daylight periods the demand peaks increase the purchase values, while when it is night the energy demand decreases and consequently the energy price. Of course, also weekly and seasonal fluctuations of electric energy price must be accounted for. These trends suggest that the conceptual design should account for price fluctuations and should also address the following dynamic issues: (i) Is it economically viable to produce electric energy within a specific chemical plant? (ii) Is it advantageous to produce electric energy by installing a dedicated plant subsection? (iii) Which are the operating steady-state conditions that maximize the profit? Specifically, the last point clarifies whether producing electric energy 24h/day is the optimal solution or the power production subsection should be operated only at some time intervals. By exploiting the enthalpy content of a hot process stream, it is possible to produce steam and electric energy. On one hand, if the hot stream does not contribute to a heat exchanger network (HEN) the energy production is always advantageous provided that the additional investment costs for the power section are counterbalanced by the operating revenues from selling the electric energy. On the other hand, if the hot stream already heats another process stream, it is necessary to uncouple them. This operation generates some operating revenues from electric energy, but it also calls for additional costs. In fact, besides the power section installation, the process requires an additional hot utility to heat the orphan cold process stream. In order to verify the feasibility of this operation through a systematic approach, we introduced the concept of dynamic superstructure. A dynamic superstructure may accept more than one alternative in the final layout (as opposed to the classic concept of superstructure, Biegler *et al.* (1997)) and by exploiting the dynamic fluctuations of prices, it allows identifying the time interval where each single process alternative should be operated. In other words, the process layout alternatives are subject to dynamic switches in order to acknowledge and exploit the external dynamic conditions of costs and prices.

3. Mathematical Formulation

The conceptual design based on dynamic superstructures calls for the solution of a mixed integer nonlinear optimization problem where the objective function is a modified and extended economic potential (EEP) according to the terminology of Douglas, 1988. A static economic potential (SEP) and a dynamic economic potential (DEP) which accounts for price fluctuations, are coupled in the objective function (1).

$$\begin{aligned} &\max_{\mathbf{x},\mathbf{y}} EEP = SEP + DEP \\ &s.t. \;\; \mathbf{h}(\mathbf{x},\mathbf{y}) = \mathbf{0} \quad \mathbf{g}(\mathbf{x},\mathbf{y}) < \mathbf{0} \end{aligned} \tag{1}$$

As far as dynamic superstructures are conceived, the discrete and Boolean variables (Bielger *et al.* (1997) allow selecting the process alternatives that can coexist in the plant, while identifying the optimal time intervals (*e.g.* hours, days, weeks, seasons) when to switch on/off them. $\mathbf{x}\in\Re^{n}$ are continuous variables and $\mathbf{y}\in\{0,1\}^{m}$ are the Boolean variables. *EEP* is the economic objective function, which summarizes investment and operating costs, and the revenues of the plant. The problem is subject to equality constraints $\mathbf{h}(\mathbf{x},\mathbf{y})$ for material, energy, and momentum balances. Inequality constraints $\mathbf{g}(\mathbf{x},\mathbf{y})$ account for quality specifications, process constraints, and law limits. The Boolean variables in the constraints set are justified by the presence of logic propositions. Nonlinearity may appear both in objective function and in constraints formulation (*e.g.* chemical equilibria, kinetics, and fluid dynamics).

Process design optimization must formulate and solve quantitatively by systematic methods the above mentioned statements. Periodic utilization of alternatives may be profitable in terms of price/cost fluctuations (*e.g.* daily electric energy market).

4. Case study

The industrial case study focuses on the layout optimization of the toluene hydrodealkylation to benzene process (Douglas, 1988). It consists mainly of a reaction zone and of a separation section. Fresh hydrogen (H_2) and toluene (C_7H_8) are preheated and fed to a plug flow reactor to produce benzene (C_6H_6). The reactor geometry must be optimized to improve the yield in benzene while reducing biphenyl ($C_{12}H_{10}$) which is a byproduct. The outlet flowrate from the reactor is first quenched and then fed to the distillation section to separate the incondensables, C_6H_6, and the low volatile components (C_7H_8 and $C_{12}H_{10}$). A gaseous H_2 (and CH_4) stream and a liquid C_7H_8 stream are both recycled to the reaction zone. A fraction of the gaseous recycle stream is purged to avoid holdup of inert components. The original layout is modified by conceiving a dynamic superstructure (Figure 1).

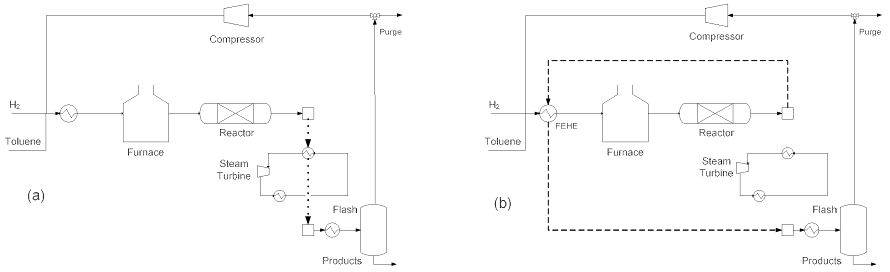

Figure 1 Daily changing process layouts. (a) daytime (b) night-time

An energy production section (EPS), which comprises a steam turbine, an evaporator and a condenser, and the feed effluent heat exchanger (FEHE) are subject to the optimization procedure, which determines whether installing or not the EPS and the time-interval of periodic operations. The simplified superstructure consists of two layouts, both capable of exploiting the enthalpy content of the outlet stream from the reactor. With reference to Figure 1, layout (a) generates electric energy by means of a dedicated plant subsection. Layout (b) preheats the flowrate entering the reactor by means of a feed effluent heat exchanger.

The decision whether to install or not the energy production section (EPS) is modeled by a Boolean variable Y that discriminates between the following alternatives: if $Y = 0$ the EPS is not economically convenient, if $Y = 1$ the EPS will be installed and operated. When $Y = 1$, besides installing the EPS, we also activate the dynamic superstructure that accounts for the coexistence of the process units devoted to the electric energy production and to the cold stream preheat. The preheat is achieved by two distinct approaches. If the EPS is not active, the hot stream can preheat the cold stream in a process-to-process heat exchanger (*e.g.* a feed-effluent heat exchanger, FEHE). If the EPS is active, the FEHE does not work (since the hot stream enthalpy is exploited in the EPS). Conversely, an additional hot utility must be used to preheat the cold stream (*e.g.* auxiliary fuel in a furnace). The optimization procedure must clarify whether the electric power production is more profitable at daytime, at nighttime, all day long, or never. In order to formalize this statement, a discrete variable, defined as the time fraction ω, is introduced in the numerical framework. This term accounts for the time-dependency of some economic factors within the process design. Specifically, ω is the ratio between the hours of energy production and the number of hours in a day. In addition, a few continuous variables $\mathbf{x}$ are introduced in the process simulation, such as the diameter of the adiabatic reactor, the purge fraction, the reactor inlet temperature, and the toluene fresh inlet flowrate. It is worth underlining that when the second alternative is active ($Y = 1$) the original feed-effluent heat exchanger requires an external duty (utility) to preheat the inlet stream to the adiabatic reactor. The overall conceptual design can be formulated as follows:

$$\max_{\mathbf{x},\mathbf{Y},\omega} EEP(\mathbf{x},\mathbf{Y},\omega) = SEP + DEP = EP_3^{steady} - CI_{heat} - CV_{furnace} +$$

$$+Y\left(P_{el}\left(p(\omega),\omega\right) - CI_{el} - CV_{heat}(\omega)\right) \qquad (2)$$

$$s.t.\ \mathbf{h}(\mathbf{x},\mathbf{Y}) = \mathbf{0} \qquad \mathbf{g}(\mathbf{x},\mathbf{Y}) < \mathbf{0}$$

where EP_3^{steady} accounts for the end-product and raw material terms, as well as the equipment installation (capital investment and operating costs). CI_{heat} summarizes the capital investments for the FEHE and the furnace. $CV_{furnace}$ accounts for the operating costs of the furnace. Y is the Boolean variable that discriminates between alternatives (a) and (b) of Figure 1. When $Y = 0$, we do not install the energy production section. Conversely, when $Y = 1$ we install the energy production section and we have to consider the time-dependency of some economic terms, *e.g.* the revenues from selling electric energy $P_{el}\left(p(\omega),\omega\right)$, and the operating costs due to purchasing the auxiliary fuel $CV_{heat}(\omega)$ to preheat the raw materials. CI_{el} quantifies the investment costs for plant expansion (*i.e.* installation of the EPS).

Figure 2 shows the daily fluctuations of electric power price in a specific day (14-Jul-2008).

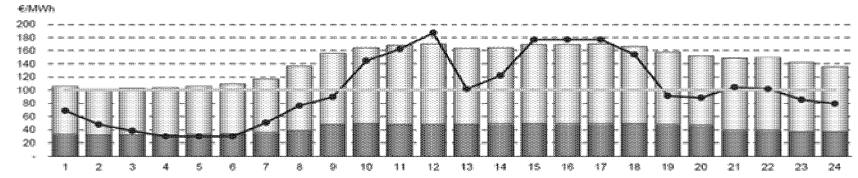

Figure 2 Italian daily energy price on 14-Jul-2008 (source: www.mercatoelettrico.org).

5. Numerical Results

PRO/II, a detailed process simulation software developed by Simsci-Esscor (Invensys), simulates the toluene hydrodealkylation process. PRO/II produces the input data for the evaluation of the economic objective function *EEP* by modeFRONTIER (Enginsoft), which is an optimization package. With reference to the optimization routine, the Multi-Membered Evolution Strategy (MMES) algorithm solved the MINLP problem. Figure 3 shows the *EEP* value as a function of the ω when the power production starts at 10:00am (circles). The triangles represent the cumulative mean of the energy price $p(\omega)$. The horizontal line is the breakeven, singling out the profitable limit. This line is obtained by setting $Y = 0$, *i.e.* by removing the energy production section. When circles are above the breakeven line of Figure 3, the economic revenue can be increased by power production. It is worth remarking that we would expect a profit higher than the breakeven point at the beginning of the diagram of Figure 3, since we chose to plot it starting from the first economically convenient time interval.

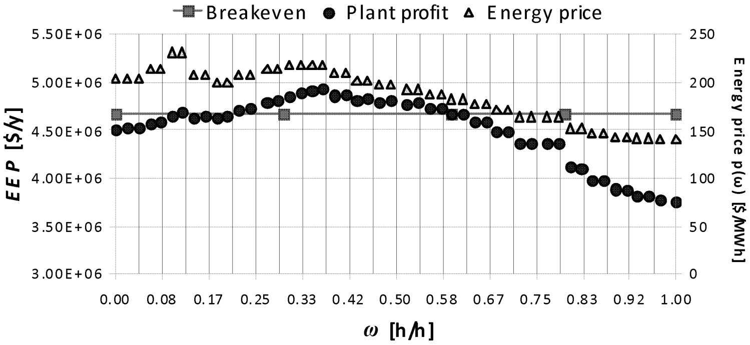

Figure 3 Extended Economic Potential (i.e. objective function) as a function of omega. Plant profit is time-dependent.

However, it is necessary to account for the investment costs related to the equipment for power generation. The first hours of energy production are necessary to refund the additional capital investment. Moreover, if we consider the cost of the fuel (hot utility) to preheat the inlet stream to the reactor (during the electric power production), the real economic margin is reduced further. Actually, the first derivative of the *EEP* respect to ω is:

$$\left.\frac{d\,EEP}{d\omega}\right|_{\mathbf{x},\mathbf{Y}} = f\left(p(\omega)\right) - q\left(c_{fuel}\right) \tag{3}$$

where $f\left(p(\omega)\right)$ depends on the energy price and consequently on ω, while $q\left(c_{fuel}\right)$ depends on the fuel cost. The net profit margin increases when the derivative of the objective function is positive, since $f\left(p(\omega)\right) > q\left(c_{fuel}\right)$. On the other hand, when the derivative becomes negative then the plant profit starts decreasing since the cost for the additional fuel required by the furnace is larger than the additional margin earned by power production (*i.e.* $q\left(c_{fuel}\right) > f\left(p(\omega)\right)$).

This means that the energy production becomes less profitable up to a condition where it assumes values that are below the breakeven line. The solution of problem (2) allowed deducing that the installation of a power generation section is economically feasible if the electric energy is produced and sold in the time interval 10:00am-06:00pm. In the remaining portion of the day, it is preferable to use the hot outlet stream from the reactor to preheat the inlet stream by means of the process-to-process FEHE.

6. Conclusions

This manuscript tried to address and discuss the influence of price/cost fluctuations on the design of chemical processes. We considered the daily market fluctuations of electric energy and we introduced the concept of *dynamic superstructure*. Dynamic superstructures allow formulating mathematically the periodic operation of some portions of a chemical plant, according to exogenous price/cost fluctuations. This approach based on a systematic method analyzes quantifies the increase of economic revenues as a function of the installation of specific process subsections. Even if no further costs are accounted for the dynamic evolution of the process (*i.e.* transient periods produced by switching from one process layout to another), the case study showed some significant conclusions about the feasibility of installing an energy production section.

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