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A combined heuristic and indicator-based methodology for design of sustainable chemical process plants

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ABSTRACT

The current emphasis on sustainable production has prompted chemical plants to minimize raw material and energy usage without compromising on economics. While computer tools are available to assist in sustainability assessment, their applications are constrained to a specific domain of the design synthesis problem. This paper outlines a design synthesis strategy that integrates two computer methodologies – ENVOP*Expert* and *SustainPro* – for simultaneous generation, analysis, evaluation, and optimization of sustainable process alternatives. ENVOP*Expert* diagnoses waste sources, identifies alternatives, and highlights trade-offs between environmental and economic objectives. This is complemented by *SustainPro* which evaluates the alternatives and screens them in-depth through indicators for profit and energy, water, and raw material usage. This results in accurate identification of the root causes, comprehensive generation of design alternatives, and effective reduction of the optimization search space. The framework is illustrated using an acetone process and a methanol and dimethyl ether production case study.

1. Introduction

Chemical industry has been the epitome of modern process industry. Its importance to the world economy is apparent with U$2.4 trillion annual sales of more than 70,000 different products, ranging from basic chemicals, specialty chemicals, life sciences, and consumer products (KPMG, 2010). Despite its importance, the general public perception of the chemical industry has not been favourable. A recent survey conducted by the European Chemical Industry Council revealed that the public rating of this industry was 49% positive and 44% negative (ICIS, 2007). Such a negative public perception is most likely due to the growing concerns over the possible ill-effects from the use of chemicals and chemical based products and the environmental damages (such as global warming, ozone depletion, etc.) caused by the pollutant emissions. For example, of the total CO_2 emission discharged to the atmosphere, about 25% can be attributed to the chemical industry (ICCA, 2009). Another main concern is associated with the large-scale processing of non-renewable resources that are typical of the chemical industry. Representing 4% of the world economy, the chemical industry is currently responsible for 7% of global energy use (Lines, 2005). In the USA, the percentage is even higher with the chemical industry accounting for nearly 25% of the energy used for industrial activity; further, 88% of this is derived from fossil fuels (National Research Council, 2005). Certainly, such level of consumption cannot be sustained in the long run. With the recent emphasis on process sustainability, much improvement is expected from the chemical industry to minimize its raw material and energy consumptions and pollutant generation without compromising the economic value of the enterprise. Responding to these challenges then requires a new insight into the characteristics of a sustainable system and a fundamental rethinking of how a chemical production plant is to be designed, built and operated (Bakshi & Fiksel, 2003).

Design is an iterative activity which requires decision making at various stages and at different levels of detail. Overall, a design activity involves accepting as input an abstract description of the desires of an organization and delivering a refined description of a concrete product, process, or system that will satisfy those desires (Cano-Ruiz & McRae, 1998). In the context of chemical process design, for example, the abstract goal can be to convert excess methanol from one plant into a dimethyl ether (DME) product. In this case, the more refined description will then be a chemical

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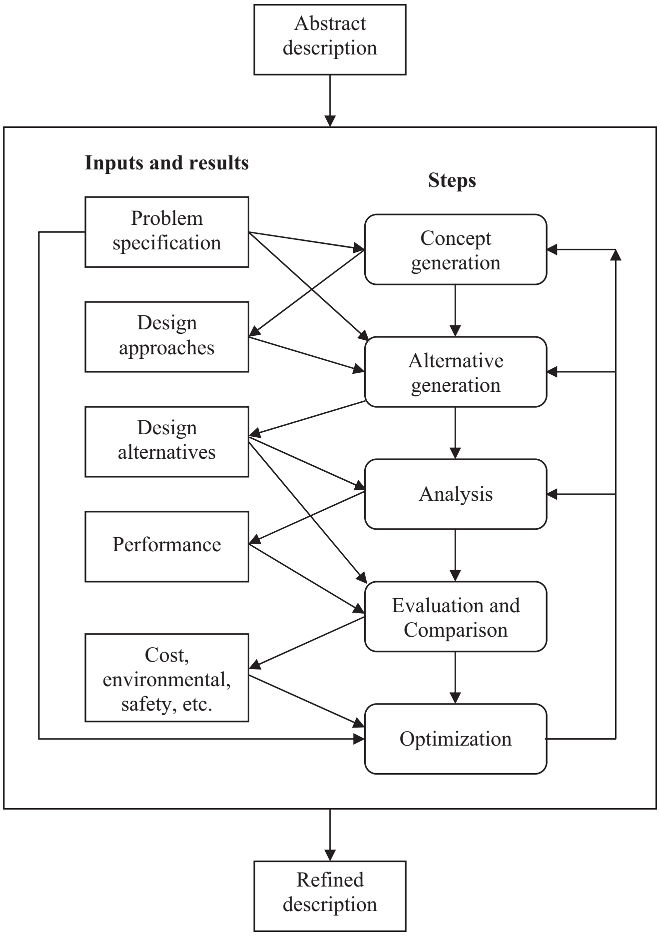

Fig. 1. Design synthesis activity (Biegler et al., 1999).

process plant to accomplish just that. Overall, such an activity of converting an abstract description into a more refined description involves a sequence of steps (see Fig. 1). The first of these steps is concept generation. Here, different concepts on which to base the design need to be identified. Typical questions to be addressed include: "should the chemistry for the methanol conversion process be based on ones found in the literature?", "should unconventional solutions be sought after?", and "should a particular design strategy (for example waste minimization as compared with end-of-pipe treatment) be adopted in the design?". Next is generation of alternatives. At this stage, different possibilities to improve the base design are considered. This is done by assessing different parts of the process to derive possible modifications to improve the process, for example, higher conversion of methanol to DME, suppression of by-products formation, and reduction of energy usage. The third is analysis of each alternative to establish its performance. Principally, this equates performing mass and energy balances of the process to determine the impacts from the alternative. The use of process simulators (such as CHEMCAD, Aspen Plus, HYSYS, PRO/II and gPROMS) will be beneficial at this stage. The fourth step involves evaluating and comparing the process performance. In this step, indicator metrics that measure the economic worth, environmental impact, safety impact, and so on need to be calculated for comparing the alternatives and shortlisting the promising ones. Finally, optimization can be performed for adjustment and refinement of the process variables to further improve the design. This optimization can be cast as a multi-objective decision problem, where trade-offs between economic, environmental, and safety concerns need to be resolved.

Design synthesis is thus a complex, laborious, time consuming, expensive and knowledge-intensive activity. The availability of computer-based tools that can perform systematic and thorough alternative generation, evaluation, and optimization altogether is very attractive since they can assist the designers in achieving the design goals at reduced time, money and efforts. Since the early 1960s, computer-based tools have been successfully deployed in the oil and chemical industries to expedite development and optimize the design and operation of integrated processes (Petrides, Koulouris, & Lagonikos, 2002). Their important roles to sustainability studies are now apparent with approximately 300 software applications (commercials and prototypes) available for deployment (Tsoka, Johns, Linke, & Kokossis, 2004). One sucessful example is process simulators which have been extensively used to compare the environmental impacts from various plant modifications (Cabezas, Bare, & Mallick, 1999; Chen & Shonnard, 2004). Building on the results of process simulators, mathematical optimization have been applied to fine-tune the decision variables controlling the process such as pressure, temperature and flow rate to simultaneously maximize the profit and minimize the environmental impact (Dantus & High, 1996; Fu, Diwekar, Young, & Cabezas, 2000). Process integration tools such as pinch-based analysis have also been successfully deployed for targeting energy and water reduction and designing heat- and mass-exchange networks (El-Halwagi, 1997; Linnhoff, 1995). Another important tool is artificial intelligence-based technique including P2TCP – a heuristic design based expert system for minimizing waste generation and energy consumption (Pennington, 1999) and ENVOP*Expert* – a combined knowledge-based and optimization system for sustainable design and operation (Halim & Srinivasan, 2011). An indicator-based computer tool, called *SustainPro*, has also been developed by Carvalho, Matos, & Gani (2008) for generation and evaluation of sustainable design alternatives. While all these tools are beneficial, their applications are limited to solving specific domains of sustainability problem, such as minimization of process or utility wastes, optimization of process variables, and generation of qualitative design alternatives. To deliver a comprehensive sustainability solution to a process, collaboration between the different tools is needed. However, such effort has proven to be challenging as each seeks to tackle the problem from a different viewpoint (Hilaly & Sikdar, 1994). For example, the analysis and evaluation methods implemented in ENVOPExpert is limited to solving waste problem. Further, a large optimization search space could result since the proposed design alternatives and decision variables for optimization are considered of equal importance to the process. In the case of SustainPro, while the alternatives proposed and decision variables can be ranked in term of potential for improvement, they are not optimized.

This paper outlines a design synthesis methodology that claims merits for integrating two computer systems – ENVOP*Expert* and *SustainPro* – for sustainable design and operation. The term "integration" here means the two systems are deployed on parallel or sequentially (depending on the step of the methodology) in a complementary fashion for process design synthesis. For this, we have also used a set of sustainability metrics defined by the Institution of Chemical Engineers (Azapagic, 2002) which measures the process sustainability in terms of economic; energy, water and material utilization; and environmental impacts. For the economic measures, profit and/or value added are used. For the environmental impact measures, instead of using the definition Azapagic, the WAR (waste reduction) algorithm proposed by Cabezas et al. (1999) is used. The rationale behind this research work is that by combining the collective strength of each tool, the benefits that can be gained would exceed those which could have been achieved individually. ENVOPExpert has the functionality of qualitative analysis of waste problem through heuristic solution and quantitative analysis through optimization algorithm. On the other hand, Sus-