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A knowledge-based simulation-optimization framework and system for sustainable process operations

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ABSTRACT

Design and operation of chemical plants involves a combination of synthesis, analysis and evaluation of alternatives. Such activities have traditionally been driven by economic factors first, followed by engineering, safety and environmental considerations. Recently, chemical companies have embraced the concept of sustainable development, entailing renewable feed materials and energy, non-toxic and biodegradable products, and waste minimization or even elimination at source. In this paper, we introduce a knowledge-based simulation-optimization framework for generating sustainable alternatives to chemical processes. The framework has been developed by combining different process systems engineering methodologies – the knowledge-based approach for identifying the root cause of waste generation, the hierarchical design method for generating alternative designs, sustainability metrics, and multi-objective optimization – into one coherent simulation-optimization framework. This is implemented as a decision-support system using Gensym's G2 and the HYSYS process simulator. We illustrate the framework and system using the HDA and biodiesel production case studies.

1. Introduction

The notion of sustainable development – "development that meets the needs of the present without compromising the ability of future generations to meet their own needs" (WCED, 1987) – has prompted numerous actions from governments, businesses, institutions, and industries worldwide to balance economic activities with environmental and social responsibilities. In Finland, for example, sustainable development has become a central element in driving the government policies towards improving the life of its citizens (Finland's Environmental Administration, 2006). In the U.S., various initiatives have been launched by technical institutions including the Institute for Sustainability (American Institute of Chemical Engineers) and the Green Chemistry Institute (American Chemical Society) to promote sustainable products and processes (Beloff & Lines, 2005). The expanding commitment of the industrial sector is also evident from their annual sustainability targets and achievements (BP, 2005; Shell, 2005). All these show the impact of sustainable development concept on various spheres of human activities.

Given their role as a large-scale provider of material goods within society, the chemical industries consume large amounts of non-renewable resources and concomitantly emit wastes. Representing 4% of the world economy, the chemical processing plants, with a global turnover of €1 841 billions and 10 million employees, is currently responsible for 7% of global energy use (Lines, 2005), and 4% of the total CO_2 emissions to the atmosphere (Jenck, Agterberg, & Droescher, 2004). They therefore, have an important role in contributing toward sustainable development. Specifically, to enhance their long-term sustainability, various environmental considerations including reducing raw material and energy usage, switching to renewable feedstock, and waste reuse and recycling needs to be implemented. Certainly, such measures would require changes to existing processes – ranging from simple modifications of the design and operation to more intrusive options such as material substitution and technology upgradation.

Several techniques can be used to identify opportunities for reducing pollutant generation as well as material and energy consumption within a process plant, including industrial ecology, life-cycle assessment (LCA), green chemistry, and waste minimization. These four techniques are not mutually exclusive but each seeks to improve the sustainability of a plant from a different perspective. At a geographical cluster level, industrial ecology is a method to improve the environmental impact of a plant through waste exchange, recycle, and reuse with other plants in the vicinity (Ehrenfeld & Gertler, 1997). One example of the successful imple-

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mentation of this technique is at the Kalundborg industrial park in Denmark (Chertow, 2000), where an oil refinery, power station, gypsum board facility, pharmaceutical plant, and the city itself, share water, steam, and electricity resources, and also exchange a variety of wastes. The outcome is a 25% reduction of the fresh water usage, 2.9 million tons of material recycling, and energy for heating 5 000 homes. LCA is a tool for elucidating the environmental burdens over the entire life-cycle of the product, starting from raw material extraction to production process, point of use, and final disposal (SETAC, 1994). Although LCA traditionally focuses on products and their impacts on the environment, it has also been applied as a decision-making tool during process design (Kniel, Delmarco, & Petrie, 1996). While industrial ecology and LCA focus outwards from the process and plant, green chemistry and waste minimization look inwards. The production process can be made inherently benign through green chemistry, which involves designing new processes or products (such as catalysts) that eliminate or reduce the use and generation of hazardous substances (Anastas & Warner, 1998). Given its nature, this is mostly applicable in the initial design stages where changes to the process chemistry are still viable. On the other hand, waste minimization is a manufacturing-centric activity which avoids, eliminates or reduces waste at its source, or allows reuse or recycling of the waste within a plant (Crittenden & Kolaczkowski, 1995). It is thus suited for initial process design as well as the retrofit situation, where different modifications can be proposed to the base case design and operation in order to improve the environmental performance.

This paper presents a knowledge-based simulation-optimization framework for generating sustainable design and operations alternatives for chemical process plants. The proposed framework, which has been implemented as a fully automated decision-support system, combines different process systems engineering (PSE) methodologies – knowledge representation, waste source diagnosis, knowledge-based design retrofitting, quantitative assessment of the alternatives and multi-objective optimization – for sustainable process operations problem. The paper is organized as follows: in the next section, we review the literature on waste minimization. In Section 3, the knowledge-based simulation-optimization based framework is proposed. The integration of the heuristic-based waste diagnosis with process simulation and mathematical optimization is described in Section 4. The development of a decision-support system that automates the various elements of the framework is also outlined. In Section 5, we illustrate the framework on a biodiesel production process.

2. Waste minimization in process plants

A number of PSE methods have been proposed to guide the non-expert in performing waste minimization. A comprehensive review of these methods is available from Cano-Ruiz and McRae (1998). In the broadest sense, the available methods can be classified into qualitative and quantitative approaches. In the qualitative approaches, process synthesis techniques such as Douglas' hierarchical procedure (Douglas, 1992), onion diagram (Smith, 1995) and Environmental Optimization, ENVOP (Isalski, 1995) can be applied to identify potential waste minimization solutions to a process. In the quantitative approaches, pinch technology (Linnhoff, 1995), mass-exchange network (El-Halwagi, 1997), superstructure optimization (Dantus & High, 1996) or simulation can be used to better integrate the process and/or its utility network. In general, the qualitative approaches are easy to use even by a non-expert. However, they only provide broad direction for improving the process. On the other hand, the quantitative approaches can provide precise actions for retrofitting. However, they need specialized expertise. In this work, we seek to link the chasm between the two, using process simulation as the bridge.

The process simulator has today become a standard tool in the repertoire of process engineers. The main advantages of the process simulator are that various process modifications can be evaluated easily using standard software packages (such as CHEMCAD, Aspen Plus, HYSYS, PRO/II and gPROMS) in a short time without the need for extensive experimentation or pilot plant testing. It has also been used for environmental studies. Dantus and High (1996) combined Aspen Plus simulator with superstructure optimization for selecting the optimal plant configuration that can reduce waste generation and energy consumption while remaining profitable. They applied their methodology to a case study involving methyl chloride production. Cabezas, Bare, and Mallick (1999) used the CHEMCAD simulator to compare the environmental impacts from various modifications made to the plant. Their objective was to reduce the environmental impact through material recycling in a methyl ethyl ketone plant and an ammonia production process. Fu, Diwekar, Young, and Cabezas (2000) combined Aspen Plus simulator with numerical methods to solve multi-objective optimization problem involving environmental impact and profit. They illustrated their methodology on a hydrodealkylation (HDA) process of toluene to produce benzene. Mata, Smith, Young, and Costa (2003) used PRO/II simulator to assess diferent design alternatives of a HDA plant. They examined the possible fugitive and open emissions from the plant and evaluated the potential environmental impacts and economics of various design options. Another similar development by Chen and Shonnard (2004) utilized the HYSYS simulator with its optimizer module to screen design alternatives for a maleic anhydride process. Recently, Othman, Repke, Wozny, and Huang (2010) used the Aspen Plus simulator, a spreadsheet and multi-criteria decision-making tool for sustainability assessment and selection of chemical process design alternatives for a biodiesel production process.

Another approach to sustainability analysis is adopted by *SustainPro* – an indicator-based approach for identifying, screening and evaluating design alternatives of chemical processes (Carvalho, Matos, & Gani, 2008). *SustainPro* uses process information in the forms of mass and energy balances from a simulator and applies a set of mass and energy indicators of Uerdingen, Gani, Fischer, and Hungerbühler (2003) and Uerdingen, Fischer, Gani, and Hungerbühler (2005) to determine design alternatives through path-flow analysis. This methodology is based on the reverse-design approach, wherein target values are assigned to indicators and the variables that are most sensitive to the indicators are identified.

One main shortcoming of the process simulator-based approaches is the lack of decision support for the non-expert user. The inherent capability of process simulators is limited to predicting the behavior of the process in response to changes in one or more variables. When used for waste minimization, the overall outcome of the study is still very much dependant on the insight, skill, and expertise of the user in diagnosing the traits of waste generation in that specific case, identifying the relevant features (root causes) that control them, exploring and generating different alternatives, and tuning the necessary variables to optimize the process. This shortcoming of the process simulator-based approaches has indeed been highlighted during a joint workshop organized by the U.S. Environmental Protection Agency, the Department of Energy, and the Center for Waste Reduction Technologies (Eisenhauer & McQueen, 1993). Their recommendation was to develop an integrated framework comprising of an expert system and process simulator. The rationale behind this is that since waste minimization is a multifaceted problem, its solution requires the application of different computational tools, each providing a different perspective. In the following, we use the term "evaluate" to mean a value is assigned while the term "analyze" refers to "examine critically, so as to bring out the essential elements" (Dictionary,