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ORIGINAL PAPER

Economic and environmental optimization of the biobutanol purification process

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Abstract Current technologies for the production of biobutanol by fermentation have improved the production processes. These new technology improvements are economically viable with respect to the petrochemical pathway. For this, the aim of this paper is to compare four different process designs for the purification of biobutanol by solving a multi-objective optimization process involving two objective functions: the total annual cost and return of investment as economic functions and the associated eco-indicator 99 as an environmental function. The process associated to the routes A, B, and C consists of a steam stripping distillation and distillation columns, while the process D includes distillation columns with a liquid–liquid extraction column. Process modeling was performed in the Aspen Plus software, and the multi-objective optimization was conducted using differential evolution with tabu list as a stochastic optimization method. Results indicate that the process route D is the most profitable design and the process route C has the lowest environmental impact measured through the eco-indicator 99 method. Additionally, the use of a solar collector against steam has been compared in order to produce the required heat duty needed in every single distillation column to have a broader view about the environmental and economic impact of these devices.

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Keywords Biobutanol separation · Economic and environmental optimization · Differential evolution with tabu list · Biofuels · Solar collector

List of symbols

ABE	Acetone–butanol–ethanol
C_{TM}	Capital cost of the plant
C_{ut}	Utility costs
DDE	Dynamic data exchange
DE	Differential evolution
DETL	Differential evolution with tabu list
D_{cn}	Column diameter
ETSC	Evacuated tube solar collector
F_{rn}	Distillate fluxes
GAs	Genetic algorithms
LLE	Liquid–liquid extraction
LCA	Life-cycle assessment
N_{tn}	Total column stages
N_{fn}	Feed stages
ROI	Return of investment
RFS	Renewable fuel standard program
R_{rn}	Reflux ratio
TAC	Total annual cost
TL	Tabu list
x_m	Vectors of required purities
y_m	Vectors of obtained purities

Introduction

During the last decades, there has been an increasing interest for renewable energy sources because of the problems associated to global warming, climate change, and volatile oil supply (Brekke 2007). Further environmental

Financial Risk Assessment and Optimal Planning of Biofuels Supply Chains under Uncertainty

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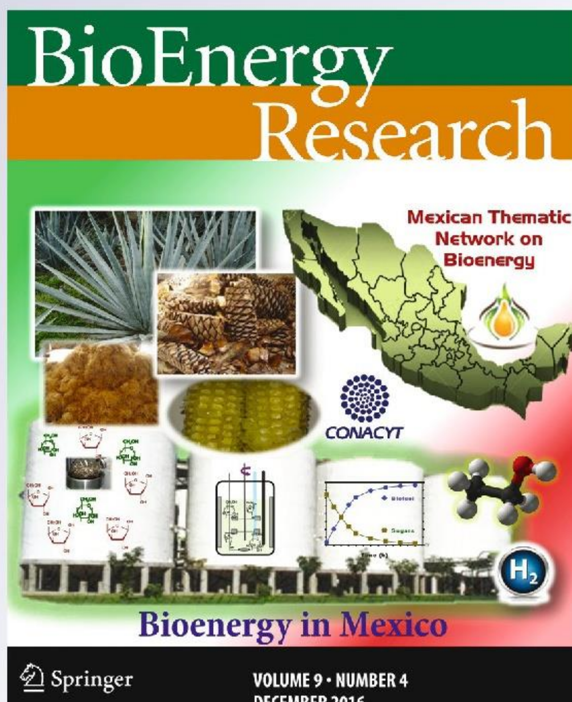

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Stochastic design of biorefinery supply chains considering economic and environmental objectives

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A B S T R A C T

Biomass is a renewable resource that has attractive characteristics for energy production, but the corresponding supply chain could be subject of several uncertain factors that can affect drastically the optimal configuration, and those have not been properly accounted in previous publications. Therefore, this work presents a new approach for the optimal planning under uncertainty for a biomass conversion system involving simultaneously economic and environmental issues. The environmental impact was measured via the Eco-indicator99 method and the economic aspect was determined through the net annual profit. The proposed method considered the uncertainty involved in the raw material price by the stochastic generation of scenarios using the Latin Hypercube method followed by the implementation of the Monte-Carlo method, where a deterministic optimization problem was solved for each single scenario to select the structure of the more robust supply chain relying on statistical data. The proposed approach was applied to a case study for a distributed biorefinery system in Mexico. The results showed that the behavior of the profit values for the stochastic case is not associated to the behavior of the raw material price; also, it is possible to observe that the supply chain topology could be affected for the uncertainty in the raw material price; however, the environmental and economic objectives did not present significant changes.

1. Introduction

In recent years, biomass has been identified as a potential renewable energy source for production of biofuels, chemicals and other high value-added products using diverse processing technologies (Ng et al., 2015). Torjai et al. (2015) have stated that a serious discussion of the use of biomass for energy production should include the entire supply chain, and Liew et al. (2014) concluded that the use of biofuels has increased in the recent years, but it is still necessary to assess their potential impact on the economy, human health and environment before they could be implemented to replace the fossil fuels. Additionally, Akbari and Karimi (2015) indicated the importance of analyzing the entire supply chain for any process. For the specific case of supply chains based on biomass, Shabani and Sowlati (2013) presented a study for a supply chain configuration based on forest biomass for producing power. Haankuku et al. (2015) proposed a mixed-integer programming model for determining the adequate price of the ethanol produced in a biorefinery, as well as the size and location of the processing plant. Moreover, a mathematical approach for the optimization of the operational decisions in the supply chain design was proposed by Yue and You (2014), and Ahn et al. (2015) developed a deterministic mathematical programming model for the strategic planning of a supply chain based on biodiesel production from microalgae.

The previous studies have considered that the biomass processing is accomplished through biorefinery systems; in this context, several works based on the biomass processing via biorefineries were discussed in a paper review published by Eskandarpour et al. (2015). It should be noted that the interest in the processing of biomass has been focused on its attractive characteristics from the social, environmental and economic points of

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AIChE

Optimal Reuse of Flowback Wastewater in Hydraulic Fracturing Including Seasonal and Environmental Constraints

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This article presents a mathematical programing formulation for the optimal management of flowback water in shale gas wells. The formulation accounts for the time-based generation of the flowback water, the options for treatment, storage, reuse, and disposal. The economic and environmental objectives are considered. The economic objective function is aimed at determining the minimum cost for the fresh water, treatment, storage, disposals, and transportation. The environmental objectives account for the fresh water usage and wastewater discharge. To carry out the water integration, a reuse network including treatment is proposed. Additionally, the model considers seasonal fluctuations in the fresh water availability. A given scheduling for the completion phases of the wells is required to implement the methodology. Finally, an example problem is presented to show the applicability of the proposed methodology. © 2016 American Institute of Chemical Engineers *AIChE J*, 62: 1634–1645, 2016

Keywords: water management optimization, shale gas, hydraulic fracturing (fracking), flowback water reuse, fresh water restrictions

Introduction

Recently, there have been substantial discoveries of shale gas reserves in North America. Hydraulic fracturing technologies have facilitated the production of shale gas trapped in tight formations. According to the Energy Information Administration (EIA), by the year 2035 shale gas is expected to provide about half of the total natural gas supply in the United States.[1] The EIA also estimates that the United States has enough natural and shale gas to meet domestic electricity demands for 575 years at current electricity generation levels. Certainly, this information highlights the importance and the enormous potential of shale gas in the future. Siirola[2] analyzed the impacts of shale gas in the chemical industry and in the natural gas market. Weijermars[3] modeled the future gas production up to 2025 in the six major shale plays of United States under uncertain conditions with the purpose of determining different scenarios of production. Cafaro and Grossmann[4] presented a model to plan the shale gas supply and to determine the number of wells, the size of gas processing plants, the section and length of pipelines for gathering raw gas and delivering processed gas and by-products, the power of gas compressors, and the amount of freshwater required from reservoirs for drilling and hydraulic fracturing so as to maximize the net present value of the project. He and You[5] integrated the shale gas processing with ethylene production to increase the profitability. Yang et al.[6] developed a new design to integrate an oil shale refinery with reforming retorting gas; this scheme allows the production of the required hydrogen in the hydrogenation step and considerable economic benefits are obtained compared with the conventional refinery process. Wang and Xu[7] proposed a new methodology for the simultaneous operation of shale gas, NGL recovery, and LNG re-gasification considering the uncertainty of the shale gas feed rate. Knudsen et al.[8] presented a mathematical formulation for well scheduling using a Lagrangian relaxation. Pirzadeh et al.[9] carried out a study for hydraulic fracturing additives, which are capable of generating H_2S under hydrothermal conditions or delaying the production of native H_2S. Furthermore, He and You[10] presented a novel process design for a greener chemicals production integrating shale gas with bioethanol dehydration and Gao and You[11] designed and planned shale gas supply chains under uncertainty including the drilling, production, processing, and transportation.

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Optimal Safe Layouts with Heat Exchanger Networks Synthesis Having Isothermal Process Streams

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This paper proposes a new MINLP model for heat exchanger network synthesis considering streams with phase change and their geographical allocation based on safety. For heat exchanging, the model includes streams with latent heat, streams with sensible heat, and streams with both latent and sensible heat. Streams may be generated in either an already installed facility or in a new facility for siting, and their point of generation inside the facility is given. For safety, the model considers the possibility of having toxic releases in either installed or for siting facilities. Hence the facilities layout becomes a part of the HEN synthesis optimization problem. A grid layout is adopted to allocate facilities in the available land and a new strategy is developed to solve the non-overlapping facilities constraint. This strategy also reduces the numerical difficulties appearing when Euclidian distances are required when calculating safety affectations.

1. Introduction

The design and synthesis of heat exchanger networks (HEN) has been substantially improved along last decades due to the high economical savings in the chemical and process industry. The design and synthesis of HEN has been largely explored and a broad research has been published in the chemical engineering literature. An early method to obtain HEN with minimum area, proposed by Hohmann (1972) and described in (Gundepsen and Naess, 1988), called the attention of several researchers. This work included a strategy to assess feasibility of streams assuming suitable approach temperature and given utility supplies. The underdeveloped technology eventually evolved into what became known as the pinch design method (Linnhoff and Hindmarsh, 1983). From a mathematical programming point of view, Grossmann and Sargent (1978) gave the first step into the MINLP developments by using an algorithm for discrete variables to solve the HEN problem with incorporated integer variables in the mathematical model. This algorithm was in fact a clever extension of the method developed by Ponton and Donaldson (1974). In particular, the concept of superstructure gave a graphical understanding of the HEN problem (Yee and Grossmann, 1990; Yee *et al*., 1990). An interesting work has increased stages in previous superstructures by calculating the number of stages based on the inlet temperatures of the hot and cold streams as well as on the exchanger minimum approach temperature (Zamora and Grossmann, 1997). An excellent review on HEN has been elaborated by Furman and Sahinidis (2002). Besides numerical improvements to solve the optimization problem, HEN research and their applications have been evolved in several directions. The operation of heat exchangers have been also included in the optimization model to provide flexibility and resilience in HEN designs (Jäschke and Skogestad, 2014). Some of the difficulties to solve during operations due to bad designs have been explored recently (Jensen and Skogestad, 2008). A mixed-integer linear model to detect the optimal set of units to be cleaned during plant maintenance has been recently developed (Assis *et al*., 2013). In general, the main purpose of HEN synthesis became the finding of optimal solutions in an efficient way, and several models were proposed to solve different conditions or scenarios. The proposed approaches have ended up in

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Life cycle assessment for Ambrox® production from different chemical routes

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ABSTRACT

Industrial processes usually have significant environmental impacts due to the emissions associated with different production processes, resource depletion, and ecosystem alteration. Since these processes are designed to meet primarily economic aspects, there arises a need to balance with social and environmental issues. Strategies such as process integration and optimization have been used to reduce the overall environmental impact through recycle and reuse of materials or via the adoption of alternative manufacturing routes which may result in enhancing the economic and/or environmental objectives. *Ambrox®* is a high value chemical used in the perfume industry. The traditional chemical processing route represents significant environmental problems. In this paper, an economic and environmental evaluation of the chemical routes from *Sclareol* (the most common chemical route) and from *Ageratina jocotepecana* (an endemic plant from the State of Michoacan in Mexico) is analyzed to determine the feasibility of using the latter as an alternative for the production of *Ambrox®*. The results are analyzed using the Life Cycle Assessment method and show that the chemical pathway from *A. jocotepecana* offers environmental and economic advantages over the current process.

1. Introduction

Fixatives are among the most important chemicals used in the perfume industry. These are intended to offer stable and long-term effects for the perfumes. In some cases, fixatives are used in ratios of nine parts of fixative to one part of essence. Because of its attractive properties, *Ambrox®* containing the compound Ambergris has been used as a key fixative in the perfume industry. Traditionally, Ambergris was obtained from intestinal excretion of sperm whales (Frater et al., 1998). More recently, alternative chemical routes have been investigated because of the animal rights issues associated with obtaining the chemical from whales (Costa et al., 2005). Until recently, the most common chemical route involved *Sclareol*, a compound obtained from the *Salvia sclarea* (*SS*) which is an herbaceous plant. This synthetic process includes 34–42 chemical stages (Barrero et al., 1993). Recently, a new chemical route from *Ageratina jocotepecana (AJ)*, an endemic plant from the State of Michoacán in Mexico, has been proposed (Gutiérrez-Pérez et al., 2012). This route reduces the chemical stages to only one chemical cyclization under mild conditions. Having only one chemical cyclization offers several technological advantages such as reducing the number of required equipment, the land occupation by the process plant, manpower, residues and energy use. Theoretically, all these aspects should yield a more sustainable process from the economic, environmental and safety points of view. Given the process simplification advantage of the *AJ* route, it is important to explore and quantify the economic and environmental performance of this route compared to the *SS* route. It is also necessary to consider the chemical synthesis pathway in the overall context of a supply chain. Recent research has highlighted the important economic and environmental implications of considering a chemical pathway in the context of its supply chain

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