



Optimal design of rainwater collecting systems for domestic use into a residential development



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ABSTRACT

This paper proposes an optimization-based approach for designing rainwater harvesting systems for domestic use in a residential development. The optimization model accounts for the implementation of rainwater harvesting devices, pipes and reservoirs for the optimal siting, collecting, storing and distribution of harvested rainwater. The optimization model consists in satisfying the water domestic demands and considers as objective function the minimization of the total annual cost associated to the fresh water, the capital costs for the catchment areas, storages and pumps, and the cost associated to the pumping, maintenance and treatment. A case study for a residential development in Morelia, Mexico is presented. The city of Morelia is characterized for having complications to satisfy the water demands, especially during dry seasons. The application of the proposed optimization approach shows that it is possible to satisfy a significant percentage of the domestic water demands using a harvesting rainwater system decreasing the associated cost in the time horizon. Several scenarios have been presented to show the potential solutions identified in the case study.

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1. Introduction

Water is one of the most valuable resources in the world; due to its vital role in life, recently the water demands have dramatically increased due to the population growth and also to the change in the precipitation patterns because of the climate change. This way, there are several highly populated regions of the world where there is water scarcity. This has motivated the development of harvesting water strategies to satisfy the water demands (Abdulla and Al-Shareef, 2009; Appan, 2000; Chilton et al., 2000). In the industry, several strategies for water reuse, recycling and regeneration have been proposed in order to satisfy specific demands and this way to reduce the consumption of freshwater (see for examples Deng and Feng, 2011; Fu et al., 2012; Ng et al., 2010; Yu et al., 2013). Particularly, mathematical programming-based techniques have represented powerful tools for the optimal design of industrial water networks reducing the fresh water consumption and the wastewater discharge to the environment (see Burgara-Montero

et al., 2012; Deng et al., 2013; Khor et al., 2012; Nápoles-Rivera et al., 2010, 2012; Ponce-Ortega et al., 2011, 2012; Rojas-Torres et al., 2012; Rubio-Castro et al., 2010, 2011, 2012, 2013; Sotelo-Pichardo et al., 2011; Vázquez-Castillo et al., 2013). On the other hand, the water consumption for domestic use represents around 10% of the total fresh water demand in the world, and satisfying these domestic demands represents a major problem in places with water scarcity. In this context, several strategies have been implemented to satisfy the domestic water demands involving rainwater harvesting as shown in Fig. 1 (see Domènech and Saurí, 2011; Domènech et al., 2012; Gikas and Angelakis, 2009; Hadadin et al., 2010; Li et al., 2010; Morales-Pinzón et al., 2012); however, these strategies have been based on heuristic approaches that frequently do not produce an optimal solution for the addressed problem. Recently, several systematic techniques to satisfy the domestic water demands based on the optimal storing and distribution for the available water have been proposed. Khastagir and Jayasuriya (2010) presented a model for the optimal sizing of tanks for rainwater with domestic purposes. Imteaz et al. (2011) presented a decision support tool for sizing rainwater tanks associated to large roofs. Liu et al. (2011) presented a mixed integer linear programming model for using desalinated water to satisfy domestic demands. Atilhan et al. (2012) presented a system-integration

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An MFA optimization approach for pollution trading considering the sustainability of the surrounded watersheds



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ABSTRACT

This paper proposes a mathematical programming model for the pollution trading among different pollution sources which considers the sustainability of the surrounding watershed. The formulation involves the minimization of the costs associated to the implementation of the required technology to satisfy the environmental constraints in order to achieve optimal water quality conditions. The model uses a material flow analysis technique to represent changes on the behavior of the watershed due to the polluted discharges. The material flow analysis considers all discharges and extractions (i.e., industrial and residential discharges, pluvial precipitation, evaporation, etc.) as well as the chemical and biochemical reactions taking place in the watershed. In the context of pollution trading, the implementation of the proposed formulation determines if an industrial source must buy credits to compensate the violation of environmental constraints, or if it requires the installation of treatment technologies to sell credits to another source. The formulation was applied to a case study involving the drainage system of the Bahr El-Baqr region in Egypt; the results show the advantages of the proposed approach in terms of cost and sustainability.

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1. Introduction

Current economic development policies must consider the sustainability of the systems under analysis. Sustainability includes environmental issues and social welfare. Important efforts have been made recently to improve the environmental quality and various environmental management policies have been implemented. The command and control policies and those programs that use economic incentives for environmental compliance, such as pollution trading, are among these strategies. The pollution trading concept is attributed to Crocker (1966), Dales (1968) and Montgomery (1972). Former applications of this market strategy have been the trading of SO_x and NO_x emissions for acid rain control (Ferral, 1991) with positive effects (Burtraw, 1996; Burtraw, Evans,

Krupnick, Palmer, & Toth, 2005; Burtraw, Krupnick, Mansur, Austin, & Farrel, 1998; Burtraw & Mansur, 1999). The benefits obtained from the implementation of this strategy are: (i) significant cost reductions related to pollutant treatment, (ii) flexibility to dischargers in meeting pollutant load reductions, (iii) creation of incentives for control beyond current limits, (iv) promotion of technological innovation and (v) investment to obtain credits and extra profits. Additional environmental benefits (such as improved wildlife and co-control of other pollutants) have also been reported (Rousseau, 2001; USEPA, 2004). This strategy has also been used in water quality control with successful results (Lal et al., 2009; Rousseau, 2001; Selman et al., 2009; Smajgl, Heckbert, Ward, & Stratton, 2009; USEPA, 2008; Woodward, 2002).

Literature reports several models to describe the trading mechanisms between pollution sources. Some of the models consider pollutant nonpoint sources (Ghosh, Ribaud, & Shortle, 2011; Luo, Maqsood, Huang, Yin, & Han, 2005; Wang, Zhang, Huang, & Li, 2004; Zhang & Wang, 2002), market equilibrium and permits (Bosetti, Carraro, & Massetti, 2009; Hung & Shaw, 2005; Innes, 2002). Also, recent works analyze the effect of more complex issues in the trading policies, such as pollutant dynamics and pollutant interactions

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Optimal design of thermal membrane distillation systems with heat integration with process plants



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HIGHLIGHTS

- An optimization model for thermal integration for seawater desalination is proposed.
- A thermal membrane distillation module is integrated with a process.
- The objective function maximizes the net annual profit.
- Results show substantial benefits.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper presents an optimization approach for the design of thermal membrane distillation (TMD) systems that are thermally coupled with processing facilities. A superstructure representation and an optimization formulation are introduced to obtain simultaneously the optimization of the TMD unit and the heat-exchange network (HEN) that integrates heating and cooling in the process facility. The superstructure and associated optimization formulation seek to identify the system configuration along with design and operating variables such as heat-exchanger areas, membrane area, extent of thermal coupling between the process and TMD, and the TMD feed-preheating temperature. The objective function maximizes the net annual profit which accounts for the revenues from the sales of purified water, the avoided cost of the treated wastewater, and the total annualized costs accounting for the capital investment of the added heat transfer units and the TMD network, the operating costs for the heating and cooling utilities and the operating expenses for the TMD system. The proposed optimization formulation is applied to a case study where a TMD system is integrated with a methanol plant and the results show significant economic benefits for the implementation of the proposed methodology.

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1. Introduction

The limited supplies of fresh water coupled with the over-exploitation of the available fresh water bodies represent major challenges for the sustainable development and call for cost-effective strategies for water management [1]. There are several regions around the world where desalination is the primary source

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Sustainable Integration of Algal Biodiesel Production with Steam Electric Power Plants for Greenhouse Gas Mitigation

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ABSTRACT: Significant reductions in anthropogenic greenhouse gas (GHG) emissions, particularly of fossil carbon dioxide (CO₂), are necessary worldwide in order to prevent adverse impacts of global climate change on the socio-economic sectors, ecological systems, and human health. In this context, this study aims to investigate the economic and environmental aspects of sustainability associated with the integration of algal biodiesel production with a steam electric power plant for microalgae biofixation of CO₂ in flue gases and then algal biomass conversion to biodiesel. This integrated energy system is a multipurpose process that provides the CO₂ required by the microalgae cultures as well as electricity, biodiesel produced from the algal biomass, and lipid-depleted biomass which is in turn used as an auxiliary fuel in the power plant. A multi-objective optimization strategy based on genetic algorithms is proposed to yield a set of optimal solutions providing the best compromise between the profit and the environmental impact of regenerative Rankine power generation plants coupled with algae-to-biodiesel production facilities. The power plant operates continuously, but CO₂ is fed to open pond raceways only during the daytime (12 h a day) for algae growth. The rigorous IAPWS-IP97 formulation is used to calculate the thermodynamic properties of water and steam in the steam power cycle. The environmental impact is measured by the Eco-indicator 99 methodology that follows LCA principles. The optimization problem includes the selection of multiple primary energy sources for the power plant boiler, such as fossil fuels (coal, oil, and natural gas), biofuels, and biomass (switchgrass, softwood, and hardwood) in order to achieve significant reductions of CO₂ emissions. The optimal trade-off designs are obtained by implementing the ϵ -constraint method. The optimization method has been applied to a case study in México. The Pareto optimal solutions indicate that the current price for biodiesel of \$3.91/gal on average would make the integrated energy system under consideration profitable. In addition, the system could achieve significant environmental improvements due to life-cycle GHG reductions that result not only from biofixation of CO₂ from combustion flue gases by microalgae and then algal biomass conversion and use as renewable fuels (i.e., biodiesel and lipid-depleted biomass) that substitute for fossil fuels, but also by significantly reducing the fossil fuel requirement compared to stand-alone coal-fired power plants.

KEYWORDS: GHG mitigation, Biological capture of CO₂, Microalgae biodiesel production, Steam power plants, Sustainable energy system, Multi-objective optimization, Life cycle assessment



INTRODUCTION

Worldwide electricity consumption is growing rapidly and is expected to rise significantly in the coming decades because of population growth and economic and social development, especially in developing countries. In fact, the International Energy Agency¹ estimated that the worldwide consumption of electricity will increase by 95.8% over the period of 2008–2035; using the reference case “current policy” scenario, it is expected to increase from 16,800 TWh to 32,900 TWh (3.55% average annual growth). For meeting this growing global demand for electricity, projections from IEA² show that fossil fuels, especially coal and natural gas, will be our main source for electricity generation in fossil fuel-fired power plants at least

over the next couple of decades. Because fossil fuel combustion power stations are responsible for over 65% of estimated carbon dioxide (CO₂) emissions caused by power generation systems,¹ a major challenge facing this electric power sector is how to reconcile the growing global electricity demand with the increasing urgency to reduce CO₂ emissions due to carbon dioxide being the main greenhouse gas (GHG) and, consequently, one of the most important contributors for the increase in anthropogenic climate change and global warming

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Optimal design of inter-plant waste energy integration



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HIGHLIGHTS

- An optimization approach for heat integration in eco-industrial parks is proposed.
- Waste heat recovery is proposed through integrated organic Rankine cycles.
- Improved energy integration schemes are obtained with the proposed approach.

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ABSTRACT

In this paper, a new superstructure for heat integration of an eco-industrial park is proposed. Intra and inter-plant heat exchange for the process streams is allowed. For a proper reuse of the waste heat at low temperature, a set of organic Rankine cycles (ORCs) can be integrated inside the eco-industrial park. This way, the proposed superstructure allows proper heat integration to reduce the use of external cooling and heating utilities as well as the consumption of external electric energy. The proposed superstructure is modeled through a mathematical programming formulation where the objective function considers the simultaneous minimization of the operating and capital costs for the units involved in the system as well as the possible revenues from the sales of electricity. The model is formulated in such a way that avoids numerical complications during its solution. Results from the application of the proposed approach show that the interplant-integration offers significant savings compared to the traditional single-plant integration with and without considering ORCs.

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1. Introduction

Energy consumption represents a major concern in industry because of the massive requirements of external utilities such as heating, cooling and electricity. In addition to the economic aspect, the use of these utilities represents a severe environmental impact because usually fossil fuels are burned to produce electricity and hot utilities. In this context, the synthesis of heat exchanger networks (HEN) has been a very attractive option to reduce the external consumption of hot and cold utilities. The main idea of the HEN synthesis is integrating the heat of process streams by allowing heat exchanges between hot process streams (streams that need to be cooled) and cold process streams (streams that need to be heated) in such a way that the overall external heating and cooling

utilities are minimized [1–4]. The selection of the allowed matches between hot and cold process streams is not trivial, and several methods have been reported to solve the synthesis of HENs. The aforementioned methods have been classified as heuristic [5–10], based on stochastic searches [11,12] and based on mathematical programming approaches [13–26]. In addition, several approaches have been reported to retrofit existing HENs [27–32]. The implementation of HENs allows reducing the external consumption of hot and cold utilities in a given plant (see Fig. 1); usually significant amounts of heat at low temperatures have to be removed using external cooling utilities [33–41]. However, this process excess heat at low temperature (i.e., waste heat) can be used as heat source for an organic Rankine cycle (ORC) to produce electric power. This way, reducing the use of external cooling utilities and, at the same time, providing part of the electric power required for the process can be achieved (see Fig. 1) [42–49]. The ORC is characterized by using an organic fluid as working fluid. In this regard, several works have focused on the selection of the working fluid, which depends

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Waste Heat Recovery through Organic Rankine Cycles in the Bioethanol Separation Process

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ABSTRACT: The huge use of heating utilities is one of the main drawbacks associated with the azeotropic separation process for the bioethanol production. In this context, process integration through heat exchanger networks can be used to integrate the involved streams; however, the main problem in this scheme is that the streams that require cooling are at lower temperature than the ones that require heating, yielding very small opportunities for energy integration. Recently, the organic Rankine cycle has been proposed as an alternative for waste heat (i.e., heat at low temperature) recovery producing electric power. Therefore, in this paper is presented an optimization study for the energy integration in the azeotropic bioethanol separation process involving energy integration through heat exchanger networks incorporated into an organic Rankine cycle. A proper optimization approach is proposed to yield the solution with the minimum separation cost. Several separation sequences are used to demonstrate that incorporation of the organic Rankine cycle to energy integration in bioethanol production yields significant economic benefits. Furthermore, this integrated scheme improves the energy efficiency for the waste heat recovery, making more attractive the use of bioethanol.

■ INTRODUCTION

Decreasing greenhouse gas emissions (GHGE) has become an important global issue because the effects of climate change have negatively affected the whole world. The main source of GHGE is the use of fossil fuels for heating, electricity generation, and transportation. One alternative to reduce these emissions is to substitute totally or partially fossil fuels with bioethanol,^{1,2} which is obtained from renewable resources. Furthermore, bioethanol can be implemented easily in the existing infrastructure and can substitute for methyl *tert*-butyl ether (MTBE) as an octane enhancer in gasoline engines.³ Nowadays, the largest bioethanol producer in the world is the United States, where bioethanol is produced mainly from corn,⁴ followed by Brazil, where the feedstock is sugar cane.⁵ However, the current methods for producing bioethanol (see Figure 1) use large amounts of energy in the separation process associated with the ethanol–water azeotropic mixture (because the ethanol–gasoline blend has low water tolerance).^{6–8} Traditionally, the separation of the ethanol–water mixture is carried out through azeotropic distillation using benzene, pentane, or diethyl ether as solvent; another alternative is extractive distillation using ethylene glycol or gasoline.^{9,10} Furthermore, these technologies involve large capital and operating costs.^{7,11–15} In addition, bioreactors usually yield low concentrations of bioethanol,^{16,17} and huge utilities are required in the process (i.e., electricity, steam, and cooling water). For these reasons, until now bioethanol has not been yet economically competitive with respect to fossil fuels.

The azeotropic distillation process for the bioethanol–water mixture has associated several hot streams that require cooling and cold streams that require heating (Figure 1).^{6–10} In this context, energy integration through heat exchanger networks can be an attractive solution for reducing the external energy

consumption in the separation process.^{18–25} Therefore, recently Vázquez-Ojeda et al.²⁶ proposed integrating energetically the process streams involved in the bioethanol separation process through the SYNHEAT model.^{27–31} The main problem with this previous approach is that in the bioethanol separation process the hot streams are at low temperature, which decreases drastically the possibility of using these streams to heat the cold process streams that are at higher temperatures. In the approach by Vázquez-Ojeda et al.²⁶ the integrated energy is low and so the reduction in the consumption of utilities. On the other hand, recently the organic Rankine cycle (ORC) has been proposed to recover waste heat and produce electric power; this unit is similar to the steam Rankine cycle (SRC), but it uses a refrigerant as working fluid.^{32–36} Desai and Bandyopadhyay³⁷ have proposed integrating an ORC to a heat exchanger network (HEN) for waste heat recovery, and then Hipólito-Valencia et al.^{38–40} proposed superstructures and mathematical programming models for waste heat recovery through ORC in the synthesis of HEN. These approaches have shown that the ORC is able to recover a significant amount of waste heat, producing electric power and yielding significant economic improvements. Therefore, this paper proposes the use of an ORC integrated to HEN for energy integration during the bioethanol separation process. In this way, several optimized separation sequences using different solvents and configurations^{24,41} are integrated energetically involving the use of an ORC and using a new method for the energy integration.

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Multiobjective Design of Interplant Trigeneration Systems

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A systematic approach for heat integration into an eco-industrial park through an integrated trigeneration system is presented. The approach is based on a new superstructure formulated as a multiobjective mixed-integer nonlinear programming model, where intraplant and interplant heat exchange for the process streams is allowed, in addition to the energy integration into the utility system that is constituted by a steam Rankine cycle (to produce electric power and hot utility), an organic Rankine cycle (to recover waste heat and produce electric power), and an absorption refrigeration cycle (to recover waste heat and provide refrigeration). To run the utility system, several external heat sources (solar, fossil fuels, and biofuels) are considered, which impact the economic, environmental, and social objectives considered in the model. A systematic approach to tradeoff the objectives considered is presented. Two examples are presented, where the advantages of the integrated eco-industrial park are shown. © 2013 American Institute of Chemical Engineers AIChE J., 60: 213–236, 2014

Keywords: energy integration, waste heat recovery, interplant integration, eco-industrial park, power plant, absorption refrigeration, trigeneration

Introduction

Currently, the enormous energy demand in the process industries has promoted the development of integrated utility systems. The chemical and process industries consume huge amounts of hot utilities (as medium/low pressure steam), cooling water, and refrigeration (absorption refrigeration for moderate temperature and mechanical refrigeration for low temperature). In this context, the integrated trigeneration system has emerged as a suited solution to integrate the process streams to the utility system (see Figure 1a); where electric power, steam, and refrigeration is produced simultaneously.

For a given process industry, there are several potential solutions to integrate the utility system; in this regard, recently several approaches for the optimal design of utility systems integrated to process streams have been proposed. Particularly, several approaches have been reported for the optimal integration of process streams to cooling water systems (e.g., Mixed Integer Non Linear Programming (MINLP) synthesis of cooling networks,¹ detailed design of cooling networks,² optimization models for recirculating cooling water systems,³ effluent cooling systems,⁴ involving multiple cooling towers,^{5,6} subambient conditions,⁷ for retro-

fitting,⁸ involving pressure drops considerations,⁹ and for targeting¹⁰). Furthermore, some approaches for the optimal integration of process streams to refrigeration systems through absorption refrigeration cycles¹¹ (ARCs) have been recently reported (integrating solar energy¹² or renewable energy¹³ and involving economic and environmental objectives¹⁴). Additionally, several approaches for the optimal integration of process streams with a steam Rankine cycle (SRC) have been reported (identifying optimal pressure levels,¹⁵ generating sustainable electric energy,¹⁶ involving multiobjective optimization,¹⁷ for targeting,¹⁸ and considering the environmental impact¹⁹); this integration usually involves the electric power production and the energy recovery from the condenser of the SRC to heat cold process streams (cogeneration). Moreover, several approaches to integrate industries with a central SRC that involve solar energy,²⁰ the utility system,²¹ H₂ production,²² reductions of fuel, power, and CO₂,²³ targeting for cogeneration potential,^{24,25} planning utility systems,²⁶ total site utility system,²⁷ exergy for targeting refrigeration,²⁸ fired heaters,²⁹ specific minimum temperature difference,³⁰ and the industrial implementation³¹ have been proposed, which has been called total site integration.³² In addition, Bagajewicz and Rodera^{33–35} and Rodera and Bagajewicz^{36,37} presented mathematical programming approaches for energy integration across plants, and Stijepovic et al.³⁸ proposed a targeting approach for waste heat recovery across plants in industrial zones. Perry et al.³⁹

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An MINLP model for the simultaneous integration of energy, mass and properties in water networks



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ABSTRACT

A model for the synthesis of water networks with a simultaneous integration of energy, mass and properties is presented. The model is formulated within a mixed-integer nonlinear programming framework where the objective function accounts for the minimization for the total annual cost satisfying energy, mass and property constraints for the water streams involved in the network. To accomplish this task, a new superstructure is proposed, in which a first stage for energy integration before mixing streams was considered, followed by a mass and property integration network, and placing finally a second energy integration network. Within this approach, the optimization model identifies when a stream can be used as a hot or a cold stream as part of the energy integration. The proposed approach was applied to two case studies, and the results show that there are significant advantages for the simultaneous implementation of the energy, mass and property integration strategies.

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1. Introduction

Process integration tools have been used to improve the economic performance of production processes and to provide more sustainable structures. Proper management of energy and water resources can be achieved by the application of energy and mass integration techniques. Energy integration was noticeably sparked by the development of the pinch point methodology, through which targets for minimum heating and cooling requirements are established, followed by a network design that meets such targets (Hohmann, 1971; Linnhoff and Flower, 1978; Umeda et al., 1978). The development of mass integration techniques was started by an extension of pinch concepts (El-Halwagi and Manousiouthakis, 1989, 1990); thus, targets for fresh sources consumption and wastewater flowrates were first established, and a design that met those targets through the transfer of pollutants from a set of rich streams to a set of lean streams was carried out. Alternative structures were then developed for mass integration, considering process equipments as sinks to design direct recycle networks (El-Halwagi et al., 1996; El-Halwagi, 1997; El-Halwagi and Spriggs, 1998). Through this framework, a mass integration network with a proper allocation, generation, transformation, and separation of streams and chemical species within the process is achieved. Specific applications for the minimization of the use of water in chemical processes have been developed (Wang and Smith, 1994; Dhote et al., 1996; Polley and Polley, 2000; El-Halwagi et al., 2003; Hallale, 2002).

An additional aspect to consider in mass and water integration networks was the fact that several environmental restrictions not only limit the concentration of chemical pollutants, but also the property levels that discharge streams pose to the environment, such as odor, color, and pH, among others. This gave rise to a new approach of mass integration based on properties (Shelley and El-Halwagi, 2000), which included the development of mixing rules based on property operators in order to estimate the resulting properties after mixing of streams. Such principles were used to develop methods based on pinch concepts for the design of networks with recycle, interception and process modifications based on properties (Eden et al., 2002; El-Halwagi et al., 2004; Kazantzi and El-Halwagi, 2005; Foo et al., 2006), as

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Siting Optimization of Facility and Unit Relocation with the Simultaneous Consideration of Economic and Safety Issues

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ABSTRACT: A general optimization model is proposed to determine the optimal plant layout with the simultaneous consideration of economic and safety aspects. An important characteristic of the proposed optimization model is that it allows the relocation of some of the existing units to reduce the risks associated with current locations. The formulation also allows the addition of new units. A multiobjective mixed-integer linear programming model (MO-MILP) is developed to determine the optimal location of new and existing units while accounting for cost and risk. The proposed model is analyzed through a case study for a hexane distillation process showing the advantages of considering the possibility of relocating units originally installed following exclusively heuristic approaches and economic criteria.

1. INTRODUCTION

Improper plant layout is one of the factors contributing to risks in the chemical process industry. There are numerous examples showing the implications of plant layout on safety. One example is the explosion in a polyethylene plant in Pasadena, TX, USA (1989) which led to 23 fatalities and an economic loss of about \$715 million; the inadequate distance between process equipment was identified as one of the main causes of this accident.¹ In this context, several researchers have proposed methodologies for the optimal facility layout. Díaz-Ovalle et al.² proposed an approach for the optimal distribution of new units in a given location with installed facilities. In this approach, the layout was selected based on the worst-case scenario with respect to the wind speed and atmospheric conditions in the case of toxic release in the facilities (new or existing). The approach also involved trade-offs between minimum distance and minimum risk, finding that the case of minimum distance provides unsafe locations whereas the minimum risk approach provides very large distances. Jung et al.³ proposed a mixed-integer linear programming (MILP) problem for the optimal location of new units in a discrete grid terrain, where the minimization for the cost accounting for the risk in each discrete grid was considered. Vázquez-Román et al.⁴ incorporated stochastic parameters regarding the wind speed and atmospheric conditions in a toxic gas release, where the approach was based on a mixed-integer nonlinear programming (MINLP) problem, finding numerical complications due to the nonconvex nature of the problem. Besides the allocation of new units, another important factor to consider is the interaction among facilities. This interaction can be considered by evaluating the interconnection risk and cost. Along those lines, Han and Weng⁵ proposed a methodology to evaluate the risk associated with the supply chain of natural gas. Other researchers (see, for examples, Paterson et al.⁶ Sanders,⁷ Papageorgiou and Rotstein,⁸ and Xu and Papageorgiou⁹) have solved the problem of facility layout,

where new units are added in an industrial complex in which some facilities are already installed. Han et al.¹⁰ presented an optimization approach for the facility layout including the minimization to the human risk. Furthermore, El-Halwagi et al.¹¹ proposed an optimization approach to include safety aspects in the optimal location and supply chain of a biorefinery. Martínez-Gómez et al.¹² incorporated safety issues in the optimal location of treatment units associated with industrial wastewater discharges.

Given the importance of economic and safety aspects, there is a need to develop systematic methodologies that simultaneously consider risk evaluation and cost assessment in plant layout. As such, the development of optimal facility layout is not a trivial task because of the trade-offs between the two contradicting objectives. Typically, larger distances between process equipment imply higher costs (piping, pumping, and wiring, etc.) and lower risk. Furthermore, the optimal facility location is also a function of the number of units that have to be located (Armour and Buffa¹³).

Currently, several methodologies associated with the calculus of the risk in the facility layout problem have been reported, and each methodology quantifies and includes the risk in different ways; however, there are not reported methodologies optimizing simultaneously through multiple objective functions (forming Pareto fronts) the risk and the cost, giving an explicit relation between the trade-offs of these two contradicting objectives. In the best case, the risk is included as a weighted cost in the objective function (minimizing the risk indirectly), or is calculated in the base of the layout obtained by optimizing the economic objective (only evaluating the risk without

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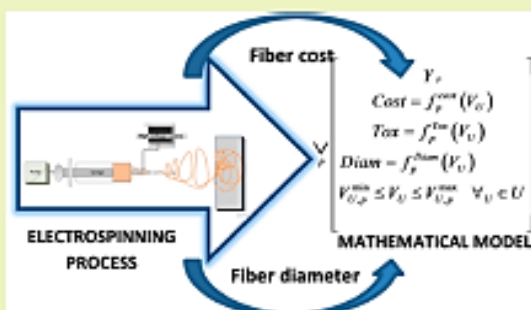
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A Mathematical Programming Approach for the Optimal Synthesis of Nanofibers through an Electrospinning Process

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ABSTRACT: This paper presents a general mathematical programming formulation to determine the optimal operating conditions to synthesize nanofibers through an electrospinning process at minimum cost. Several relationships based on experimental data for different polymers to determine the nanofiber diameter and costs are proposed. Also, a general optimization approach is proposed to trade off the relationships between cost and nanofiber diameter. A case study including the specific relationships for three polymers and five operating conditions is presented. The proposed approach is general, and it can be applied to different cases.



KEYWORDS: Optimization, Electrospinning Nanofibers, Minimum cost and diameter, Disjunctive programming

■ INTRODUCTION

Recently, the optimal synthesis of nanofibers has been the subject of several research efforts. This is because nanofibers have a high potential to be used in biomedical applications due to their high surface area with respect to their volume and microporous structure.^{1–10} Besides that, a recent market research report from BCC Research shows that nanofibers are currently the fastest growing segment of the nanotechnology market. Their market value was \$151.5 million in 2012, and the forecast is \$570.2 billion in 2017. Currently, there are several techniques available for the synthesis of nanofibers (i.e., electrospinning, self-assembly, melt spinning, template synthesis, electroblowing, and phase separation). Of these, electrospinning is the most widely studied technique and also is the most promising for tissue engineering applications.^{11–25} In the electrospinning process (Figure 1), a polymer solution is pumped at a constant rate through a syringe with a small-diameter needle that is connected to a high-voltage source, and an electric field is created between the needle and the metallic collecting plate. The solvent is evaporated before reaching the collector, and the final collected product is a mat composed of interconnected fibers. The morphology and fiber diameters produced by electrospinning are key parameters for potential biomedical applications.^{26,27} Different parameters influence the electrospinning process to yield nanofibers from polymer solutions,^{28,29–32} and several studies have focused on analyzing the effect of these parameters. In this regard, Thompson et al.³³ found that the volumetric charge density, distance from nozzle to collector, initial jet/orifice radius, relaxation time, and

viscosity have the most significant effect on the jet radius and therefore the final fiber diameter, whereas other parameters such as initial polymer concentration, solution density, electric potential, perturbation frequency, and solvent vapor pressure have moderate effects. Tiwari et al.¹² evaluated the effect of viscosity in the electrospinning process. Heikkilä et al.¹⁵ utilized an orthogonal experimental design in the electrospinning process using Polyamide-6; the analyzed parameters were polymer grade, viscosity of solution, salt content, solvent grade, voltage, distance, nozzle size, and feeding pressure of solution. In this study, the viscosity of the solution was the main parameter influencing the fiber diameters, while the salt content and strength of the electric field had strong effects. Maleki et al.²¹ implemented a genetic algorithm for analyzing the electrospinning process to determine the optimum nanofiber diameter; in this approach, the initial polymer concentration, jet radius, electrical potential, relaxation time, initial elongation, viscosity, and distance between nozzle and collector were analyzed. Sencadas et al.²⁸ evaluated the parameters in the electrospinning process to synthesize nanofibers from chitosan. Kong et al.²⁹ determined the interaction between some parameters in the electrospinning process. Torres-Giner et al.²⁹ studied the effect of molecular weight, polymer concentration, TPA/DCM ratio of solvents, and distance between the nozzle tip and the collector on the morphology

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Optimal design of process energy systems integrating sustainable considerations



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ABSTRACT

In this paper is presented a novel approach for designing sustainable trigeneration systems (i.e., heating, cooling and power generation cycles) integrated with heat exchanger networks and accounting simultaneously for economic, environmental and social issues. The trigeneration system is comprised of steam and organic Rankine cycles and an absorption refrigeration cycle. Multiple sustainable energy sources such as solar energy, biofuels and fossil fuels are considered to drive the steam Rankine cycle. The model is aimed to select the optimal working fluid to operate the organic Rankine cycle and to determine the optimal system to operate the absorption refrigeration cycle. The residual energy available in the steam Rankine cycle and/or the process excess heat can be employed to run both the organic Rankine cycle and the absorption refrigeration cycle to produce electricity and refrigeration below the ambient temperature, respectively. Two example problems are presented to show the applicability of the proposed methodology.

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1. Introduction

Nowadays energy is one of the most important resources and at the same time one of the most relevant concerns around the world owing to fast depletion of non-renewable fuels, the global warming and the climate change. For these reasons, several governments have promoted the use of cleaner energies through tax credits and there have been invested significant economic resources to searching for alternative energies to mitigate the environmental issues [1]. In this sense, power plants and industries consume enormous amounts of fossil fuels to satisfy the electricity and utilities demands. Since few decades ago, several researches prioritized this topic and focused their investigations on the maximization of recovery process heat through the minimization of external utilities using HENs (heat exchanger networks), where there are some streams requiring cooling and others needing heating (see the paper review by Morar and Agachi [2]). Nonetheless, previous approaches have been concentrated in

synthesizing HENs without considering the energy interactions among the HEN and the associated utility system.

Moreover, nowadays there are significant environmental, economic and social concerns about the utility systems; this mainly associated to the depletion of natural resources, socio-economic development and global climate change due to GHGE (greenhouse gas emissions), especially CO₂ emissions associated with the use of fossil fuels. Furthermore, when the economic and environmental criteria are prioritized together with social aspects, sustainable processes are generated. Recently, industrial processes have been addressed to consider the three aspects of sustainability for a holistic development. In this context, significant socio-economic and environmental benefits can be achieved through the optimal synthesis of trigeneration systems (i.e., cogeneration systems for combined heat, cooling and power production) that are integrated with HEN and use renewable energy resources as primary heat sources to reduce fossil fuel consumption and GHGE. Therefore, the objective of this paper is to present a mathematical formulation for the simultaneous synthesis of sustainable trigeneration systems and HEN, where the optimal working fluid to operate the ORC (organic Rankine cycle) is determined as well as the optimal system to run the AR (absorption refrigeration) cycle, considering the energy interaction among the different subsystems

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Optimum Heat Storage Design for Solar-Driven Absorption Refrigerators Integrated with Heat Exchanger Networks

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A methodology is presented for optimizing hybrid renewable energy-fossil fuel systems with short-term heat storage. The considered system is an absorption-refrigeration (AR) cycle integrated with a heat exchanger network (HEN) requiring cooling below ambient temperature. The AR cycle can be driven by multiple energy sources including excess energy from hot process streams, renewable energy sources (solar and biofuels), and fossil fuels. A two-step approach based on mixed integer nonlinear programming methods is used for the optimization. First, the problem of optimal energy integration in the hybrid energy system without heat storage is solved on a monthly basis by minimizing simultaneously the total annual cost and the overall greenhouse gas emissions. In the second step, the multi-tank thermal energy storage (TES) design problem is solved. The design involves the identification of the optimal number of storage tanks, their sizes, configuration and operation policies. The TES optimization is carried out on an hourly basis while incorporating the design targets determined by the first step. © 2013 American Institute of Chemical Engineers AIChE J, 60: 909–930, 2014

Keywords: heat integration, renewable energy, solar energy storage, multitank liquid water TES, heat exchanger network, absorption refrigerator, sustainable systems

Introduction

Nowadays one of the most important problems around the world is the proper use of energy because of the current depletion of nonrenewable fuels as well as the environmental issues generated when fossil fuels are used. Consequently, there is a need to replace fossil fuels with cleaner forms of energy (i.e., biofuels, solar energy, wind energy, etc.) but, at the same time, it is required to obtain economic benefits. This situation has promoted that a growing number of governments around the world have encouraged the use of clean energies through tax credits. In this sense, the chemical and petrochemical industry is now interested in using cleaner forms of energy because this is one of the most important energy consumers, which typically is obtained from fossil fuels with the aforementioned problems that require to be properly addressed.

Waste heat from hot process streams in industrial plants is removed by using different types of cooling systems. Above ambient temperature, the recirculating cooling water system is the most common method to remove the process waste heat. Several methodologies have been reported in the literature

for obtaining the optimal design of these heat rejection systems (i.e., Kim and Smith¹ designed a cooling system considering all the components and the interactions between cooling water networks and the tower performance; Picón-Núñez et al.² introduced a methodology for designing coolers including piping costs, exchanger costs and pumping costs; Costinovic et al.³ presented an approach for the systematic performance analysis of a cooling water system; Ponce-Ortega et al.⁴ proposed an optimization for the simultaneous synthesis and detailed design of recirculating cooling water systems; Ponce-Ortega et al.⁵ incorporated a disjunctive programming formulation for the optimal design of cooling water systems; Ponce-Ortega et al.⁶ reported a MINLP model for synthesizing cooling networks; and Rubio-Castro et al.⁷ addressed a systematic approach for the synthesis of recirculating cooling water systems involving detailed design of cooling towers, and Rubio-Castro et al.⁸ applied this approach for reducing the temperatures of hot aqueous effluent streams). On the other hand, vapor-compression refrigeration systems are commonly used to remove heat from process streams at subambient temperatures. However, these refrigeration systems involve high operating costs and very expensive compressors. Absorption refrigeration (AR) cycles are an attractive alternative to mechanical refrigeration technologies to provide the necessary cooling over moderate low temperature levels at

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Sustainable Integration of Trigeneration Systems with Heat Exchanger Networks

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ABSTRACT: A novel superstructure-based approach for synthesizing sustainable trigeneration systems (i.e., heating, cooling, and power generation cycles) integrated with heat exchanger networks is presented in this paper. The trigeneration system accounts for steam and organic Rankine cycles and an absorption refrigeration cycle. The steam Rankine cycle can be driven by multiple primary energy sources (i.e., solar, biofuels, and fossil fuels) for sustainable generation of power and process heating. The waste energy from the steam Rankine cycle and/or the excess of process heat can be used to drive both the organic Rankine cycle and the absorption refrigeration cycle to produce power and process cooling below the ambient temperature, respectively. The synthesis problem is formulated as a multiobjective mixed-integer nonlinear programming problem for the simultaneous consideration of the economic, environmental, and social dimensions of sustainability. Two example problems are presented to show the applicability of the proposed methodology.

1. INTRODUCTION

Nowadays there are several energy problems around the world such as the depletion of nonrenewable fuels, as well as the global warming and the climate change caused by the greenhouse gas emissions (GHGE) released to the environment from the combustion of fossil fuels (i.e., oil, coal, and natural gas). Currently the cheapest way to obtain energy is from fossil fuels, and several governments have promoted the use of cleaner forms of energy (i.e., solar, wind, biofuels, waste process heat, etc.) through tax credits.

Utility systems (i.e., combined cooling, heating, and power) are widely used in industrial processes to meet the heating, cooling, and electricity demands (see Figure 1), where usually fossil fuels are burned. To reduce the consumption of external utilities, heat exchanger networks (HENs) have been implemented to maximize the recovery of process heat by exchanging it between hot process streams (HPS) that have to be cooled and cold process streams (CPS) that have to be heated.^{1–4} The methodologies for synthesizing HENs have been widely classified as sequential approaches based on pinch analysis,^{5,6} stochastic methods,^{7–9} and mathematical programming based techniques.^{10–13} It should be noted that the above-mentioned methodologies have been concentrated on the synthesis of stand-alone HENs and have not taken into account the interactions between the HEN and the utility system. To address the problem of heat and power integration with the industrial processes, a number of methods have been reported in the literature. Some of them are based on thermodynamic principles and heuristic rules,^{14,15} and others use optimization techniques.^{16–18} In addition, total site analysis, which is an extension of pinch analysis, has played an important role in solving the problem of heat and power integration in a set of processes served by a central utility system.^{19–23} Furthermore, nonlinear targeting

models to get the maximum economic savings integrating heat pumps in total sites were presented by Bagajewicz and Barbaro.²⁴ For processes that operate above ambient temperature, normally recirculating cooling water systems are used to provide the required cooling utility. Recently, some works have considered the cooling tower design together with the synthesis of the associated HEN or cooling water network to properly take into account their interactions.^{25–28} Also, for processes that require below ambient cooling, Ponce-Ortega et al.²⁹ and Lira-Barragán et al.³⁰ published mathematical programming based approaches to address the problem of multiobjective optimization of absorption refrigeration (AR) cycles that are integrated with HENs.

Traditionally, the economic, environmental, and social dimensions of sustainability^{31,32} have not been simultaneously considered to evaluate the performance of industrial processes. In recent years, different multiobjective optimization approaches that only include economic and environmental aspects have been proposed to solve different engineering problems.^{33–38} Then, some works have balanced simultaneously the economic, environmental, and social objectives.^{39–41}

It should be noticed that significant socio-economic and environmental benefits can be achieved through the optimal synthesis of trigeneration systems (i.e., cogeneration systems combining heat, cooling, and power production) that are integrated with HENs and use renewable energy resources as primary heat sources to reduce fossil fuel consumption and GHGE. Therefore, the objective of this paper is to present a

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Siting Optimization of Facility and Unit Relocation with the Simultaneous Consideration of Economic and Safety Issues

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ABSTRACT: A general optimization model is proposed to determine the optimal plant layout with the simultaneous consideration of economic and safety aspects. An important characteristic of the proposed optimization model is that it allows the relocation of some of the existing units to reduce the risks associated with current locations. The formulation also allows the addition of new units. A multiobjective mixed-integer linear programming model (MO-MILP) is developed to determine the optimal location of new and existing units while accounting for cost and risk. The proposed model is analyzed through a case study for a hexane distillation process showing the advantages of considering the possibility of relocating units originally installed following exclusively heuristic approaches and economic criteria.

1. INTRODUCTION

Improper plant layout is one of the factors contributing to risks in the chemical process industry. There are numerous examples showing the implications of plant layout on safety. One example is the explosion in a polyethylene plant in Pasadena, TX, USA (1989) which led to 23 fatalities and an economic loss of about \$715 million; the inadequate distance between process equipment was identified as one of the main causes of this accident.¹ In this context, several researchers have proposed methodologies for the optimal facility layout. Díaz-Ovalle et al.² proposed an approach for the optimal distribution of new units in a given location with installed facilities. In this approach, the layout was selected based on the worst-case scenario with respect to the wind speed and atmospheric conditions in the case of toxic release in the facilities (new or existing). The approach also involved trade-offs between minimum distance and minimum risk, finding that the case of minimum distance provides unsafe locations whereas the minimum risk approach provides very large distances. Jung et al.³ proposed a mixed-integer linear programming (MILP) problem for the optimal location of new units in a discrete grid terrain, where the minimization for the cost accounting for the risk in each discrete grid was considered. Vázquez-Román et al.⁴ incorporated stochastic parameters regarding the wind speed and atmospheric conditions in a toxic gas release, where the approach was based on a mixed-integer nonlinear programming (MINLP) problem, finding numerical complications due to the nonconvex nature of the problem. Besides the allocation of new units, another important factor to consider is the interaction among facilities. This interaction can be considered by evaluating the interconnection risk and cost. Along those lines, Han and Weng⁵ proposed a methodology to evaluate the risk associated with the supply chain of natural gas. Other researchers (see, for examples, Paterson et al.,⁶ Sanders,⁷ Papageorgiou and Rotstein,⁸ and Xu and Papageorgiou⁹) have solved the problem of facility layout,

where new units are added in an industrial complex in which some facilities are already installed. Han et al.¹⁰ presented an optimization approach for the facility layout including the minimization to the human risk. Furthermore, El-Halwagi et al.¹¹ proposed an optimization approach to include safety aspects in the optimal location and supply chain of a biorefinery. Martínez-Gómez et al.¹² incorporated safety issues in the optimal location of treatment units associated with industrial wastewater discharges.

Given the importance of economic and safety aspects, there is a need to develop systematic methodologies that simultaneously consider risk evaluation and cost assessment in plant layout. As such, the development of optimal facility layout is not a trivial task because of the trade-offs between the two contradicting objectives. Typically, larger distances between process equipment imply higher costs (piping, pumping, and wiring, etc.) and lower risk. Furthermore, the optimal facility location is also a function of the number of units that have to be located (Armour and Buffa¹³).

Currently, several methodologies associated with the calculus of the risk in the facility layout problem have been reported, and each methodology quantifies and includes the risk in different ways; however, there are not reported methodologies optimizing simultaneously through multiple objective functions (forming Pareto fronts) the risk and the cost, giving an explicit relation between the trade-offs of these two contradicting objectives. In the best case, the risk is included as a weighted cost in the objective function (minimizing the risk indirectly), or is calculated in the base of the layout obtained by optimizing the economic objective (only evaluating the risk without

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Optimization of facility location and reallocation in an industrial plant through a multi-annual framework accounting for economic and safety issues



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ABSTRACT

The industrial layout traditionally has been addressed accounting for the facilities distribution and installation since the first day of operation of the plant; this is, without considering future expansions that involve additional facilities in the future operation years. This way, this paper proposes a mathematical programming formulation for the optimal facility siting and reallocation in an industry accounting for future expansions and involving simultaneously economic and safety objectives. The proposed formulation is based on a multi-annual framework and this corresponds to a multi-objective mixed integer linear programming problem. The proposed optimization approach was applied to a case study for the facility siting (office buildings and control rooms) in an ethylene oxide plant. The economic objective function involves the minimization of the total annual cost accounting for the value of the money through the time and the safety objective function involves the minimization for the accumulated risk over the operation time. Results show the applicability of the proposed approach.

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1. Introduction

During the last decades several accidents have occurred in industrial facilities, which have represented several fatalities and high economic losses. The inadequate facility layout has been identified as one of the most important causes of such accidents. Usually, the techno-economic aspect has been the main factor considered in the selection of the layout of a plant, where short distances commonly are preferred because low costs for piping, pumping and interconnection. In this context, Jayakumar and Reklaitis (1994) proposed an approach for optimizing the plant layout via graph partitioning for a single level, which was then extended for multiple levels by Jayakumar and Reklaitis (1996). Georgiadis and Macchietto (1997) proposed a formal optimization approach for layout process plants. Papageorgiou and Rotstein (1998) presented a mathematical model for the optimal plant layout involving continuous domains. Georgiadis et al. (1999) reported a mathematical programming approach for process plant

layout. Penteado and Gric (1996) reported a mixed-integer nonlinear programming optimization approach for safe process plant layout. Patsiatzis and Papageorgiou (2002) reported an optimization model for multi-floor process plant layout, which was then improved by Patsiatzis and Papageorgiou (2003). Guirardello and Swaney (2005) incorporated the pipe routing in the plant layout optimization. Park et al. (2011) reported a mathematical model for the optimal multi-floor plant layout involving safety distances. The main disadvantage for these layouts is the high associated risk; this is because of the short distance between dangerous units and the high number of workers that can be affected by an accident. To overcome previous limitation, recently some methodologies have been proposed for the facility layout accounting simultaneously for economic and safety aspects. In this context, Patsiatzis et al. (2004) reported a mixed-integer linear programming model to safe process plant layout. Grossel (2004) reported some guidelines for facility siting and layout for chemical plants accounting for safety issues. Taylor (2006) incorporated safety issues in modeling LNG facility siting. Tugnoli et al. (2008a) reported an approach for safety assessment in plant layout, which was then applied by Tugnoli et al. (2008). Diaz-Ovalle et al. (2009) reported a study for comparing deterministic versus stochastic

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A Multiobjective Optimization Approach for the Development of a Sustainable Supply Chain of a New Fixative in the Perfume Industry

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ABSTRACT: Ambrox is an important fixative used in the manufacture of perfumes. It is obtained through complex chemical synthesis routes with high costs. Recent research efforts at the Institute of Chemical and Biological Researches at the Universidad Michoacana have led to the one-step synthesis of Ambrox from extracts of *Ageratina jacoitepecana* (an endemic plant of the State of Michoacán in Mexico). This new chemical route is attractive from a manufacturing perspective. However, there are several challenges for the industrial application of this plant and its incorporation in the supply chain of the perfume industry. This paper presents a multiobjective optimization approach for the development and assessment of the supply chain of *Ageratina jacoitepecana* to account for its growth in current and reclaimed lands, distribution, processing to yield Ambrox, and distribution of products. The approach accounts for the economic, environmental, and social aspects and establishes systematic trade-offs. A case study is solved to consider the supply chain and the trade-offs of the multiple objectives.

KEYWORDS: Ambrox, *Ageratina jacoitepecana*, Perfume industry, Optimization, Supply chain



INTRODUCTION

The three main components of a perfume are fragrant oils, fixatives, and solvents. A fixative is a material with low volatility that provides the long-term scent, aides in mixing with the other materials, and extends the shelf life of the perfume.¹ The fixatives are typically expensive ingredients of the perfume.¹ A commonly used fixative is *Ambergris*, which is a waxy material produced in the digestive systems of certain whale species (*Physeter macrocephalus*). Because of the limited supply of *Ambergris* and its relatively high cost, synthetic alternatives have been considered. A particularly effective synthetic fixative substitute, is *Ambrox* ((-)-8 α -12-dihydroxy-13,14,15,16-tetranorlabdane).^{2,3} The chemical structure is shown in Figure 1.

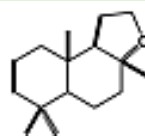


Figure 1. Chemical structure of Ambrox.

All the chemical routes reported to synthesize Ambrox involve several chemical steps having high processing costs, long reaction times, and severe processing conditions such as high pressure and temperature.^{1,4–7} These routes pose challenges for profitability and manufacturing safety. Recently, *Ageratina jacoitepecana*, an endemic plant of the State of Michoacán in Mexico, has been characterized to contain labdane diterpenes that are precursors of Ambrox.⁸ Furthermore, *A. jacoitepecana* extracts also contain (-)-8 α -12-dihydroxy-13,14,15,16-tetranorlabdane, which is a direct precursor for the synthesis of Ambrox because it requires only one reaction (chemical cyclization) to obtain Ambrox (Figure 2).⁹

The preparation of Ambrox by the chemical cyclization of (-)-8 α -12-dihydroxy-13,14,15,16-tetranorlabdane obtained from the stems of *A. jacoitepecana* offers several advantages over current chemical synthesis routes, reducing the synthesis to only one step under mild conditions and high conversion rates. Thus, it is important to determine, at least preliminary, if it has

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Multiple Steady States in Thermally Coupled Distillation Sequences: Revisiting the Design, Energy Optimization, and Control

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Supporting Information

ABSTRACT: The design, optimization, and control of thermally coupled distillation sequences with side columns have been extensively studied in the literature. Energy savings of up to 30% have been reported for such systems; further, dynamic simulations show that the theoretical control properties and closed-loop dynamic responses of thermally coupled distillation sequences are better than those of the conventional distillation sequences. In this paper, we have extended the optimization search for the energy required on the separation of a ternary mixture, detecting two feasible solutions for the energy required in the reboiler for the same value of the interconnecting stream (multiple steady states), filling the gap about this topic on these systems. The multiple steady states detected in the thermally coupled distillation sequences (TCDS) were subjected to a controllability analysis and a closed-loop dynamic study. According to the controllability analysis, the steady state with higher demand of energy in the reboiler presented better theoretical control properties than those of the steady state with lower energy requirement in the reboiler. Consistent with the controllability results, when the two steady states were studied under closed-loop using PI controllers, the best dynamic responses for set point tracking and load rejection were exhibited by the steady state design with the higher energy requirement in the reboiler.

1. INTRODUCTION

Because distillation is an industrial operation with high energy demand and a very low thermodynamic efficiency,^{1,2} several studies have been conducted in order to mitigate those problems. Tedder and Rudd¹ presented a very complete study of the energy requirements of eight distillation sequences for the separation of ternary mixtures. They compared complex distillation sequences, including the thermally coupled distillation sequences (TCDS) with side columns, against the classical direct and indirect distillation sequences, obtaining energy savings of around 30% by using the TCDS with side columns in comparison to conventional distillation sequences for ternary mixtures (A,B,C) with low content of the intermediate component.

Glinos and Malone³ estimated the amount of vapor generated in the reboiler under minimum reflux conditions for complex and conventional distillation sequences. They concluded that savings of around 30% in the minimum vapor generated in the reboilers were achieved by using TCDS with side columns.

Several studies have reported that TCDS can reduce capital costs and energy requirements in the range between 30% and 50% in comparison to the conventional distillation sequences.^{4–7}

Despite the energy savings achieved in the complex distillation sequences, it was thought that their control and operation could be more difficult than in the conventional distillation sequences due to the presence of recycle streams. However, posterior studies evaluated their control properties^{8–11} and showed that their control properties were as good as those of the conventional distillation sequences and similar closed-loop dynamic responses were presented.

Recently, it has been reported that TCDS and reactive distillation systems can show steady state multiplicity due to their complex physicochemical behavior.^{12–14} In the case of finding multiple steady states, a control properties analysis can help to select those operational parameters that result in the best dynamic performance. In this work, comparative studies are conducted on the theoretical control properties and closed-loop dynamics responses for set point tracking and load rejection for some steady states found within the regions of multiplicity in the TCDS systems; then, these studies allow us to select the best steady state in terms of cost and control. This is significant since these kinds of complex distillation sequences

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