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Short Communication

Design and optimization of an ethanol dehydration process using stochastic methods

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ABSTRACT

Due to the increasing demand for renewable fuels that are economically attractive, as well as part of the quest for energy alternatives to replace carbon-based fuels, the purification of ethanol plays a key role. This paper presents the design and optimization of a dehydration process for ethanol, using two separation sequences: a conventional arrangement and an alternative arrangement based on liquid–liquid extraction. Both sequences were optimized using a stochastic global optimization algorithm (differential evolution) implemented in Mathworks Matlab and coupled to rigorous process simulations carried out in Aspen Plus. The economic feasibility of the two configurations was studied by changing the ethanol–water composition in the analyzed feed stream. The results clearly demonstrate that significant savings are possible by extraction when the ethanol content in the feed stream exceeds 10% mol (22 wt%).

1. Introduction

Ethanol is by far the most promising sustainable biofuel, with major advantages over all other fuel alternatives (such as hydrogen) – as it can be easily integrated in the existing fuel systems as a 5–85% mixture with gasoline that does not need any modification of the current engines. Brazil and United States are major users and producers of bioethanol, and as such both countries together were responsible for 88% of the world's ethanol fuel production in 2010. Remarkable, bioethanol is an environmentally-friendly fuel with less greenhouse gases emissions than gasoline, but with similar energy power [1].

The bioethanol production at industrial scale relies on several processes, such as: corn-to-ethanol, sugarcane-to-ethanol, basic and integrated lignocellulosic biomass-to-ethanol. However, according to Pimentel [2], the corn and other food crops should be used for food as priority and not for ethanol production. The ethanol production is claimed to increase the degradation of the environment as the corn production causes more soil erosion than any other crop. Moreover, it can take more than 29% of energy to produce one gallon of ethanol, as compared to the energy content of a gallon of ethanol. According to these and also other factors, it was concluded that ethanol production from subsidized US corn is in fact not a renewable energy source. Nigam and Singh [3] performed a review of all the available literature up to date concerning liquid biofuels. Although biofuels seem not to be yet an economical alternative to large-scale biofuel supply, there is still an urgent need to perform extensive research in order to introduce more efficient processes by developing the technology, reducing the energy requirements, decreasing emissions and production costs, and ultimately establishing biofuels as an alternative for the future. Anhydrous ethanol is widely used in the chemical industry as a raw material in chemical synthesis of esters and ethers, and as solvent in production of cosmetics, sprays, perfumery, paints, medicines and food, among others. The most popular processes used in ethanol dehydration are: heterogeneous azeotropic distillation using solvents such as benzene, pentane, iso-octane and cyclohexane; extractive distillation with solvents and salts as entrainers; adsorption with molecular sieves; and, processes that use pervaporation membranes [1]. The large-scale production is still dominated by the extractive and azeotropic distillation despite recent advances in pervaporation and adsorption with molecular sieves [4]. The large-scale production of bioethanol fuel requires energy demanding distillation steps to concentrate the diluted streams from the fermentation step and to overcome the azeotropic behavior of the ethanol–water mixture. The conventional separation sequence consists of three distillation columns performing several tasks with high energy penalties: first a column for the pre-concentration of

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ethanol, second a column for extractive distillation and a third column for solvent recovery (Fig. 1). Considering the high costs of the ethanol dehydration, an optimization of the process is performed – where the designs of distillation and extractive distillation are usually characterized as being of large size problems, since the significant number of strongly nonlinear equations. Note that typically ethanol is pre-concentrated using a conventional distillation column to values close to the azeotrope of ethanol and water (about 95 wt% ethanol), followed by an extractive distillation column where the desired purity (over 99.8 wt% according to the standards) is achieved for ethanol, and a solvent recovery column.

Huang et al. [5] provide a review of separation process and technologies related to biorefining including pre-extraction of hemicellulose and other value-added chemicals, detoxification of fermentation hydrolyzates, and ethanol product separation and dehydration. With respect to the azeotropic nature of ethanol–water mixture they conclude that desired processes with low energy consumption are the extractive distillation with ionic liquids and hyperbranched polymers, adsorption with molecular sieve and bio-based adsorbents. New configurations have been studied for the separation process of bioethanol, such as arrangements based on thermally coupled columns and column sections recombination to obtain sequences with significant savings in the capital cost compared to the classic arrangement proposed in the literature [6]. It is also possible to reduce costs by energy integration, studies carried out in extractive distillation column using a partial condenser (the steam is fed to the second column) thus reducing the usage of steam and cooling water [7]. The alternative proposed here is to replace the distillation column used conventionally by a liquid–liquid extraction column, followed by a distillation column to recover the solvent employed. In this work we designed and optimized the process of bioethanol dehydration using the conventional process (Fig. 1) as well as the alternative separation process based on liquid–liquid extraction (Fig. 2). Moreover, different solvents [8,9] were also evaluated in the liquid–liquid extraction column, while ethylene glycol was used as extractive agent in the extractive distillation (ED). The design and optimization was carried out using, as a design tool, a differential evolution algorithm with restrictions coupled with the process simulator Aspen Plus, for the evaluation of the objective function, ensuring that all results obtained are rigorous. In this context, stochastic optimization methods are playing an important role because they are generally robust numerical tools that present a reasonable computational effort in the optimization of multivariable functions; they are also applicable to unknown structure problems, requiring only calculations of the objective function, and can be used with all models without problem reformulation [10,11].

2. Approach and methodology

Recently, the bioethanol dehydration has been studied for concentrations of 5–10 wt% of ethanol from the fermentation step, by extractive and azeotropic distillation in dividing-wall columns that are able to concentrate and dehydrate bioethanol in a single unit [4,12]. These sequences were optimized using sequential quadratic programming (SQP) method. The results show energy savings around 10% and 20% [4,12]. Ahmetovic et al. [13] presented the optimization of a plant producing corn-based ethanol, aimed to reduce the energy requirements, the fresh water consumption and the discharge of wastewater. The optimization was performed using mathematical programming techniques to optimize the energy requirements and the network for the process water. Čuček et al. [14] carried out the integration of different technologies, raw materials and energy for the dry milling process to produce ethanol from corn and stover. The optimization was performed using mathematical programming techniques using the process simulator MIPSYN. In terms of extractive distillation several authors have studied the vapor–liquid equilibrium in a ternary mixture of ethanol–water and a solvent. Wang et al. [15] measured the vapor pressure in water–ethanol mixtures, water–methanol and ethanol–methanol in the presence of an ionic liquid. García-Herreros et al. [16] have recently reported the optimization of the extractive distillation of ethanol using glycerol as an alterna-

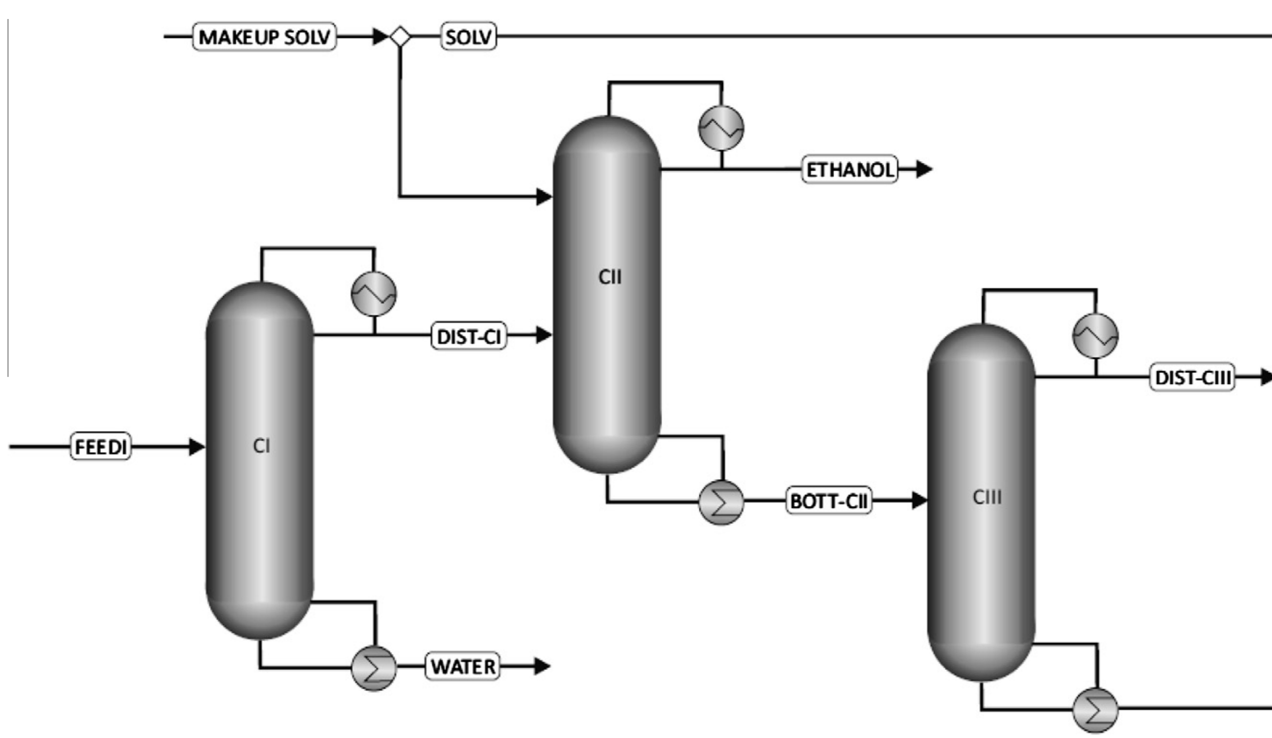

Fig. 1. Conventional separation sequence (CSS).