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Design of dividing wall columns for butanol recovery in a thermochemical biomass to butanol process

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ABSTRACT

In this work, ternary and quaternary dividing wall column (DWC) configurations for the separation of a multicomponent feed stream from a novel thermochemical lignocellulosic biomass to butanol process are designed, modeled and assessed. The goal is to separate the feed into four major products, with a key product being a biobutanol rich stream. Due to the complexity of DWC models, a shortcut modeling approach based on the minimum energy mountain method (also called the "V_{min} diagram method") is used to determine good initial values for the decision variables for the rigorous simulation of the DWC configurations. Furthermore, each DWC configuration is optimized to minimize the total annualized cost with the use of a derivative free algorithm coupled with a process simulator. The results show that the quaternary DWC configuration achieves up to 31% energy savings, and 15% capital savings in comparison to a conventional distillation sequence, and is thus a better option for implementation in the biofuel process.

1. Introduction

As a result of global efforts to reduce emissions related to fossil fuel consumption, there has been a shift of focus to produce fuels from biomass. For example, the contribution of biofuels to total road-transport fuel demand was 3% in 2013 and is estimated to grow to 8% by 2035 [1]. However, to encourage further increase in the uptake of biofuels, production costs have to be reduced. One way to address this challenge is to reduce biofuel processing costs by employing cutting edge process intensification technologies such as dividing wall columns (DWC).

Since its first industrial application in 1985 by BASF, there have been more than one hundred DWCs implemented in industry, highlighting its increasing popularity [2], with past research showing that DWCs can reduce the investment and energy consumption of a multicomponent distillation process by up to 30% in comparison to conventional distillation sequences [3–5].

Though DWC technology initially found wide application for distillation of zeotropic mixtures, its use has been further extended to other areas such as extractive distillation [6,7], azeotropic distillation [7,8] and reactive distillation [7]. Also critical to this uptake of DWCs is the fact that questions surrounding the controllability and operability of 3-product and 4-product DWCs have largely been addressed [4,9–12].

One important biofuel production process which may potentially benefit from the application of DWC technology is biobutanol production. This is because biobutanol, a gasoline substitute, is gathering increasing attention due to its advantages over bioethanol [13,14]. Recently, Okoli and Adams [15] showed that the fuel can be produced at a cost of $0.83/L using a novel thermochemical process. That process used a train of conventional distillation columns in the separation section to separate an eleven component feed into four product blends (including a fuel-grade biobutanol product), and consumed 10% of the total energy and 8% of the total direct costs of the process. However, these energy and capital costs of the separation section can potentially be improved by utilizing DWCs for biobutanol recovery instead of conventional distillation columns, leading to a reduction in production costs of the process and thus have a significant impact in improving the competitiveness of biobutanol as a gasoline replacement. This application of DWC technology has not been previously investigated for biobutanol recovery from a thermochemical process, and is an interesting area of research as past research has demonstrated the benefits of DWC applications to bioethanol, bioDME and biodiesel production processes [16,17].

Abbreviations: DWC, dividing wall columns; GA, genetic algorithm; HK, heavy key; LK, light key; MESH, material equilibrium summation and heat; MINLP, Mixed Integer Nonlinear Programming; NRTL, non random two liquid; PSO, particle swarm optimization; TAC, total annualized cost; VBA, Visual Basic for Applications; VLE, vapor liquid equilibrium; V_{min}, minimum energy mountain.

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Nomenclature

B	Bottoms flow rate (kmol/hr)
BR	Boilup ratios
D	Distillate (kmol/hr)
Dia	Column diameter (m)
f	Annualization factor
F	Feed flowrate (kmol/hr)
H	Column height (m)
i	Fractional interest rate per year
L_B	Liquid flow at the bottom of the column (kmol/hr)
L_T	Liquid flow at the top of the column (kmol/hr)
n	Annualization period in years (yr)
N_{feed}	Tray number of feed location
N_j	Number of trays in the jth section of the product column
N_{min}	Minimum number of trays
NT	Number of trays
q	Feed quality, liquid fraction
Q_{cond}	Condenser duty (MW)
Q_{reb}	Reboiler duty (MW)
r_L	Liquid split ratio
r_V	Vapor split ratio
RR	Reflux ratios
s	Tray spacing (m)
T_{cond}	Condenser temperature (°C)
T_{reb}	Reboiler temperature (°C)
V_B	Vapor flow at the bottom of the column (kmol/hr)
V_T	Vapor flow in the top section of the column (kmol/hr)
z	Composition

One major challenge in the research of DWC applications is their design. In commercial chemical process simulators the modeling of a DWC can be a difficult task as there are no custom DWC blocks. Methods identified from literature have made use of multiple columns in process simulators to represent different sections of the DWC [18,19]. Another challenge is the large number of internal column specifications needed for a DWC. This complexity means that computational difficulties should be avoided by using appropriate short-cut methods to determine initial estimates for the variables required for rigorous simulations. Once these variables have been estimated, rigorous simulations based on tray-by-tray MESH (material, equilibrium, summation and heat) equations can be implemented in the process simulation software. One such short-cut method is the minimum energy mountain method (also called the "V_{min} diagram method"). The V_{min} diagram method is a distillation column design tool that can be adapted and used to obtain good estimates for initializing rigorous DWC simulations. It provides a graphical visualization of the minimum energy required for separation of a multicomponent zeotropic feed as a function of the feed properties [20]. The minimum energy is represented by the normalized vapor flow in the top section of the column, with the highest peak representing the minimum theoretical energy required for separation. The concept of the V_{min} diagram was introduced by Halvorsen and Skogestad of the Norwegian University of Science and Technology (NTNU) in a series of papers in 2003 [20–22]. The method was developed based on Underwood's equations, and requires only input feed details such as feed flowrate (F), composition (z) and feed quality (q) to estimate the minimum vapor flow in the top section of the column (V_T), and distillate (D) at infinite number of trays for desired product recoveries. The method can also be used to generate initial estimates for nonideal systems by using a process simulator and a large number of trays, typically around four times the minimum number of trays (N_{min}) [20].

Outside NTNU, this method has only been applied to the design of 4-product DWCs for multicomponent aromatics mixtures [19,23] and Sun and Bi [24] to the conceptual design of 3-product reactive DWCs. These papers demonstrated the efficacy of this method. However, as the number of applications of this method is limited, more independent validations are needed to demonstrate its potential.

In process design, the comparison of different design options is usually done based on identical criteria after an optimization has been carried out. Classical methods for optimizing DWCs are based on mathematical programming (which require derivative information) and fall into a class of problems known as Mixed Integer Nonlinear Programming (MINLP) problems. This is due to the presence of discrete variables such as feed location, and number of trays in different column sections, as well as the nonconvexity of the MESH equations. Javaloyes-Antón et al. [25], reviewed the application of MINLP formulations for the solutions of complex distillation columns (including DWCs), and concluded that based on the high nonlinearities of these formulations, as well as sophisticated initialization techniques needed to obtain feasible solutions (only local optima are guaranteed as the solutions are highly dependent on the initialization points), these methods are complex and suited only for those skilled enough to adapt them for their own requirements.

An alternative, and easier to implement approach to these methods is to leverage the use of commercial process simulators and derivative-free or "black box" optimization algorithms. These derivative-free algorithms are typically population based, wherein the population contains individuals, with each individual representing a particular solution to the optimization problem. Once an algorithm termination criterion has been reached the optimization problem solution is chosen as that of the individual with the best objective function value. The advantage of these algorithms over derivative search methods is their ability to escape local optima and infeasibility regions, as well as provide multiple feasible solutions to account for real world considerations that are harder to quantify by the designer in an optimization setting. However, they are not able to guarantee that the solutions found are optimal. Though derivative-based search methods can theoretically offer local optimality guarantees, they are not easily amenable to highly complex real world problems and might be unable to find solutions which are as good as those obtained by derivative-free algorithms [25,26]. Examples of these derivative-free algorithms include genetic algorithms (GA), simulated annealing, particle swarm optimization (PSO) among others. In-depth discussions about these methods can be found in books, such as those written by Gendreau and Potvin [27], and Kaveh [28].

As a result of these advantages of derivative-free optimization algorithms over classical derivative search methods, the use of derivative-free optimization algorithms coupled with process simulators has found wide use in the literature for optimizing complicated process systems [25]. Among many examples in literature, Leboreiro and Acevedo [26] successfully demonstrated the use of a modified GA interconnected with the Aspen Plus process simulator to optimize complex distillation sequences including a Petlyuk column. Pascall and Adams [29] made use of a PSO algorithm connected to Aspen Dynamics to optimize a novel semicontinuous system for the separation of DME from methanol and water. In that work PSO was used to optimize the controller tuning parameters of the system. The PSO algorithm coupled with Aspen Hysys was used by Javaloyes-Antón et al. [25] for the optimal design of conventional and complex distillation processes. In their work, the PSO algorithm implemented in MATLAB handles all the discrete variables such as the feed location and the number