

Optimization of an Extractive Dividing Wall Column Using Genetic Algorithms

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Abstract

This work proposes an extractive dividing wall distillation column, optimal designs for which are obtained through a constrained stochastic multiobjective optimization technique. The stochastic procedure allows manipulate 15 variables simultaneously; six are continuous and the rest of them are integer. All resulting optimal designs are rigorous, since the optimization procedure is coupled to Aspen PlusTM. Several case studies are used to show the feasibility of performing extractive separations in dividing wall distillation columns. The numerical performance shows that this method appears to be robust and suitable in the design of intensified distillation systems (with dividing wall).

Keywords: dividing wall column, energy savings, optimization, genetic algorithms.

1. Introduction

Data from the United States Department of Energy indicate that distillation columns in the U.S. consume 5.07 million TJ per year; this is 43% of the total net installed capacity of the 439 nuclear power plants in operation worldwide (Plesu et al., 2008). It is clear that the main disadvantage of distillation columns is their high energy consumptions. Motivated by the large energy requirements of distillation, researchers have developed several column arrangements that can bring savings in both energy and capital cost. Reported studies reveal that the fully thermally coupled distillation system (also called the Petlyuk column) provides the maximum energy reduction in distillation columns. In most cases, this is implemented in the form of a dividing wall column (DWC), in which both columns are installed in a single shell. This reduces investment cost by 25%, operating cost by 35%, and space requirements by 40%, as compared to the conventional column system (Schultz et al., 2002). Azeotropic and low-relative volatility mixtures are commonly encountered in the fine-chemical and specialty industries, and many chemical processes depend on efficient and economical methods for their separation. These mixtures can be separated in a distillation column by altering

relative volatilities or shifting the azeotropic point to a more favorable position. Extractive distillation is defined as distillation in the presence of a miscible, high-boiling, and relatively non-volatile component, the solvent, which forms no azeotrope with the other components in the mixture. The method of extractive distillation uses a separation solvent, which is generally nonvolatile, has a high boiling point and is miscible with the mixture, but does not form an azeotropic mixture. The solvent interacts differently with the components of the mixture, thereby causing their relative volatilities to change. The optimization of a complex distillation system (as extractive distillation) is usually characterized as being of large problem size, since the tremendous number of strongly nonlinear equations results in serious difficulty in solving the model. By consequence, its solving with local optimization methods is not reliable because they generally converge to local optimums. During the last years, the development and application of deterministic and stochastic global optimization strategies have increased in many areas of Chemical Engineering. Particularly, genetic algorithms optimization methods are very attractive for engineering applications due to its reliability and simplicity in numerical implementation. Moreover, in 2008 Hernández studied the separation of a typical mixture of ethanol and water from a fermentation process. The results show that the extractive dividing wall column can produce energy savings of ca. 30% in comparison to a conventional extractive distillation column. Then, studies must be done on the complex extractive distillation systems relating to optimal design and optimization. In this study we analyze the feasibility of separating different mixtures using an extractive dividing wall column, EDWC, Figure 1. The design and optimization were carried out using, as a design tool, a multi-objective genetic algorithm with restrictions coupled with the process simulator Aspen Plus™, for the evaluation of the objective function, ensuring that all results obtained are rigorous. To the best of our knowledge, multiobjective stochastic methods have not been reported for process design of extractive dividing wall columns. The numerical performance shows that this method appears to be robust and suitable in the design of extractive dividing wall columns.

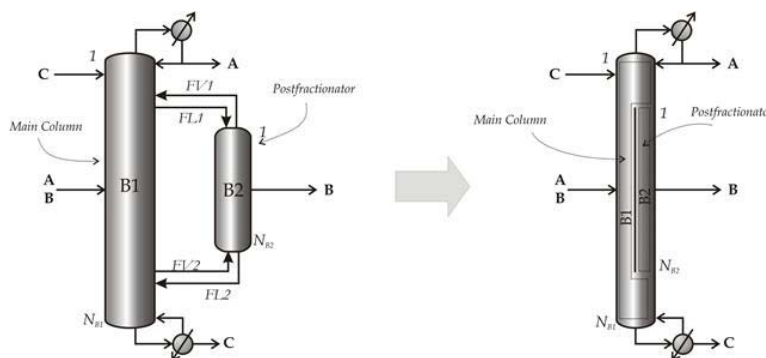


Figure 1. Extractive dividing wall distillation column (EDWC).

2. Optimization methodology

The objectives of the optimization problem for the design of extractive dividing wall columns include minimization of total number of stages on both sides of the shell (main

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column and postfractionator according to Figure 1, the extracting agent flow, and the heat duty of the sequence, but constrained by the desired purities and recoveries, i.e.:

$$\begin{aligned} \text{Min } (Q_i, N_i, F_{EA}) &= f(R_i, N_i, N_{F,i}, F_{EA}, F_k, N_k, F_{PS,o}) \\ \text{subject to} & \\ \bar{y}_m &\geq \bar{x}_m \end{aligned} \quad (1)$$

where R_i is the reflux ratio, $N_{F,i}$ is the number of the feed stage and N_i is the number of stages of column i of the sequence, F_{EA} is the extracting agent flow, F_k and N_k are the value and location of the interconnection flow k . Also, the product stream flows, $F_{PS,o}$, are manipulated, due to this also being required to manage the recoveries of the components along with their purities; \bar{y}_m and \bar{x}_m are the vectors of obtained and required purities and recoveries for the m components, respectively. In the extractive dividing wall distillation column there are four objectives to minimize: the number of stages in each side of the shell, the extracting agent flow, and the heat duty of the sequence. For these sequences the objectives are in competition, so they have to be optimized simultaneously. The manipulated variables include reflux ratio, total number of stages, the stage number and value of liquid and vapor interconnection flows, product streams flows, and extracting agent flow. The multiobjective genetic algorithm works as follows: For each run, a feasible initial design of the EDWC is given as initial solution to the algorithm; from this initial solution the algorithm generates N individuals to make up the initial population. The manipulated variables of each of the N individuals are sent to Aspen Plus to perform the simulation; then, the algorithm retrieves, from Aspen Plus, the values of objective functions and constraints for each individual. With the retrieved information the population is divided in subpopulations according to the number of satisfied constraints; at this time, the best individuals are those that satisfy the c constraints, followed by those individuals that reach $c-1$ constraints, and so on. At the end, a set of non-dominated optimal designs of the extractive dividing wall distillation columns are obtained. More details of the method can be found in Gutiérrez-Antonio and Briones-Ramírez (2009).

3. Case of study

Optimal designs of the extractive dividing wall distillation columns were obtained for four binary mixtures with different extracting agents (Table 1). For the extractive dividing wall distillation sequences we used 2500 individuals and 40 generations as parameters of the genetic algorithm, with 0.80 and 0.05 of crossover and mutation fraction. Phase equilibrium of these mixtures is calculated with the solution model UNIQUAC for all mixtures. For all mixtures studied, the purities and recoveries were fixed at 99% for the compositions of the products and the extracting agent.

Table 1. Mixtures analyzed.

Mixture	Feed components	Extracting agent	Feed Flow, (kgmol/h)	Feed composition (Mol fraction)
M1	n-Heptane/Toluene	Aniline	181.43	0.5/0.5
M2	Tetrahydrofuran/Water	1,2-Propanediol	45.35	0.9/0.1
M3	Isopropyl alcohol/Water	Dimethyl sulfoxide	45.35	0.5/0.5
M4	Acetone/Water	Octanoic acid	45.35	0.5/0.5

4. Results

In this section we analyze the resulting Pareto fronts of the extractive dividing wall distillation columns for the different mixtures studied. We begin with a detailed analysis of mixture M1. For M1 we calculate the Pareto front using, as design tool, the multiobjective aforementioned genetic algorithm. Figure 2 shows the Pareto front for mixture 1, which includes the objectives to minimize: heat duty of the sequence, extracting agent flow, and the number of stages on both sides of the shell. The first observation is that a dividing wall distillation column can perform an extractive separation, proof of this are the 25 optimal designs that made up the Pareto front. These optimal designs satisfy the specified purities and recoveries with different structures and solvent flows, but always with the lowest energy possible. Thus, the engineer can choose the best design for his particular needs.

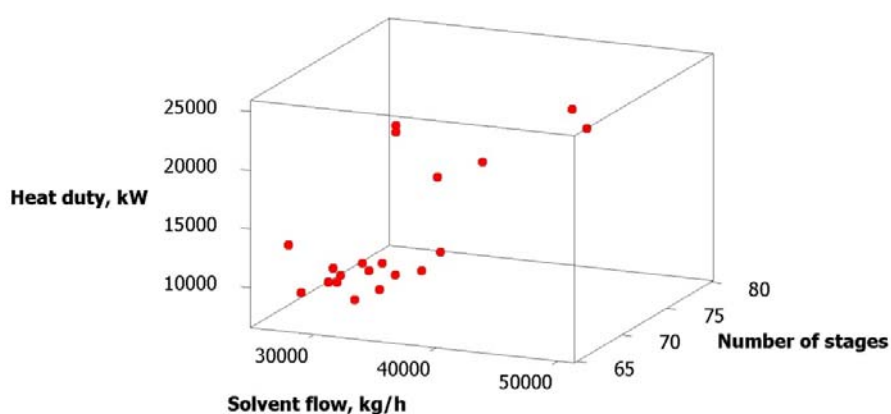


Figure 2. Pareto front of extractive dividing wall distillation columns for mixture M1.

Each design in the Pareto front is an optimal design, and this set includes designs from minimum number of stages to minimum reflux ratio, along with all designs between these extremes. Also, from this figure we can observe a good diversity in the designs that made up the Pareto front; solvent flows, number of stages and heat duties cover a wide range of values. Now, with respect to the structure of the main column of all optimal designs of the Pareto front, we can easily observe that the proportions between the different stages are kept when the number of stages of the main column is increased. From this figure, we can easily observe linear relationships between the different feed and product flows. Also, we notice that, in spite of the size of the postfractionator varying considerably, the location of the side stream stage is kept nearly constant. Thus, the size of the postfractionator varies, but the separation performed is the same for all cases. In the main column, (first side of the shell) the total number of stages varies around 53, with 51 and 57 as the lowest and highest values, respectively. On the other hand, in the postfractionator (second side of the shell), the number of stages varies considerably, from 12 to 28; in other words, this means that the size of main column remains almost constant, while the Pareto front is made up of with the variations in the structure of the postfractionator. Moreover, the ratio of flows extracting agent/feed varies from 1.55 to 2.95, with 1.88 being the average ratio, which means that, in spite of all the interconnection flows, the ratio value does not increase considerably; therefore, competitive operating costs can be expected. Also, it appears that the interconnection

flows of optimal designs present a linear relationship between one another. Finally, it was found that the optimum energy consumption design can be related to the minimum total annual operating cost (calculated using the method of Guthrie), minimum greenhouse gas emissions, and higher thermodynamic efficiencies. We clearly observe with the increase in solvent flow and total number of stages, the total annual cost also increases. From all designs of the Pareto front, we have selected the optimal design of lowest total annual cost and the one of lowest CO₂ emissions. In Table 2, we can observe that, for this mixture, the optimal design represents the lowest annual cost and the lowest greenhouse gas emissions. The thermodynamic efficiency of this sequence is 23.70%, which is slightly higher than the efficiency of a conventional extractive sequence, 21.42%; this value was obtained from an optimization of a conventional sequence only for comparative purposes. It is therefore important to remark that the thermodynamic efficiency of the extractive coupled system is slightly higher than the conventional one.

Table 2. Optimal design of the extractive dividing wall column with lowest total annual cost and lowest greenhouse gas emissions, M1.

Design variable	Value
Operating pressure (atm)	1.0
Reflux ratio in column B1	5.84
Number of stages of column B1	56
Number of stages of column B2	19
Feed stage in column B1	33
Feed stage of the extractive agent	15
Stage of the interconnection flow FV1	22
Stage of the interconnection flow FV2	44
Thermodynamic efficiency (%)	23.70
CO ₂ emissions (kg/h)	2,128.42
Total annual cost (\$/year)	2,477,452.78

With respect to the structure of the dividing wall columns, in the case of mixtures M2-M4, we found tendencies in the location of interconnection and feed streams. For all mixtures, we observe that the exiting streams are always located at the extremes of the columns, with all the feeds between them. After the FL1 interconnection flow, the first stream leaving the column, the solvent flow is present. Locations of FL2, FV1 and feed are always between the solvent flow stage and FV2 interconnection flow. The distribution of the interconnection and feed flows obeys the basic principle of increasing the interaction between the mixture and the solvent as long as possible; this is the reason why the exit flows are located at the ends of the column. In the postfractionator, the location of the side stream with respect to the number of stages is the same for all optimal Pareto front designs; the size of the postfractionator varies, but since the specifications of the separation are the same, the ratio of number of stages remains unchanged. The range for the minimum-maximum ratio of the solvent/feed flows oscillates around [1.5-2.2], [1.6-3.5] and [1.5-2.5] for mixtures M2, M3, and M4. These ratios show that the presence of four interconnection flows does not necessarily increase the solvent flow; therefore, competitive operating costs can be expected. Moreover, for all mixtures we found linear relationships between the interconnection vapor and liquid

flows. The ratio between FV2 and FV1 oscillates around 1.5 for mixtures M1, M2, and M3, but for mixture M4 this value is around 3.2. The value of this ratio depends on the modified nature of the mixture, after the addition of the extracting agent.

5. Conclusions

In this study, a multiobjective stochastic procedure is presented to obtain optimal designs of extractive dividing wall distillation columns. The stochastic procedure allows manipulation of 15 variables simultaneously; six being continuous and the rest being integer. All resulting optimal designs are rigorous, since the optimization procedure is coupled to Aspen Plus. The results show that dividing wall distillation columns are a feasible option to separate extractive mixtures, despite their highly non-ideal nature. The Pareto fronts obtained for extractive dividing wall distillation columns present good diversity, in terms of the different structures of the columns, and also with respect to energy consumption. Moreover, it was found that the optimum energy consumption design can be related to the minimum total annual operating cost, minimum greenhouse gas emissions, and higher thermodynamic efficiencies. The Pareto front is obtained from keeping constant the structure of the main column, and varying the size of the postfractionator; this behavior is because the hard separation is preferably performed in the main column. The design of the main column remains almost constant; however, the postfractionator structure varies considerably. In general, the ratio of solvent flows with respect to feed is around 1.6, inside the range recommended by the heuristic rule for conventional extractive sequences. For all cases, there are linear relationships between the interconnection flows of the dividing wall distillation columns.

6. Acknowledgements

The financial support of this work provided by Universidad de Guanajuato, Instituto Tecnológico de Aguascalientes, CONCyTEG and CONACyT (Mexico) is gratefully acknowledged.

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