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Research Article

Optimal Designs of Multiple Dividing Wall Columns

Since the optimal design of dividing wall columns (DWC) is a highly nonlinear and multivariable problem, an appropriate solving tool is required. In this paper a multi-objective genetic algorithm with restrictions is considered to design columns with dividing walls. Also, a methodology is proposed for sizing the DWC. The proposed design methodology allows achieving appropriate designs for columns with two dividing walls. As expected, the physical structures that allow the use of one or two dividing walls are not so different from each other and, as a consequence, the difference in the total annual costs for both systems depends mainly on the energy requirements.

Keywords: Design systems, Distillation, Process optimization

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1 Introduction

Distillation is one of the most used separation processes in the chemical industry, mainly because of its relative simplicity and the existent knowledge about its design and performance. The main disadvantage of this separation process lies in its high external energy input required to fulfill the desired purification. The energy requirements are provided by steam, the cost of which usually makes a high contribution to the total annual cost (TAC) of a distillation column. As an attempt to reduce the energy requirements in distillation sequences, complex structures such as thermally coupled distillation sequences have been developed. Thermally coupled sequences use vapor-liquid interconnections, allowing heat transfer by direct contact between the internal streams of the columns, thus eliminating condensers and/or reboilers of the columns. When the operating conditions are properly chosen, these systems can produce important energy savings compared with conventional distillation sequences. For ternary mixtures, the Petlyuk column has been specially studied by many researchers [1–6]. It has been demonstrated that this sequence has energy savings of about 30 % over conventional schemes [2, 7, 8]. Energy savings in a Petlyuk system exist mainly for mixtures with a low feed content of the middle-boiling component and/or when there is a symmetric distribution of the light and heavy components [9].

Considering the hydraulic issues shown by the Petlyuk sequence (because of the mismatch on the pressure profiles in the prefractionator and the main column), a thermodynamic equivalent system is used in practical applications, namely the dividing wall column (DWC). This kind of structure offers some advantages over the Petlyuk scheme. First of all, the separation takes place in one single shell; thus, the capital costs are significantly reduced. It has been reported that the use of a DWC may lead to up to 30 % reduction in the capital costs [10–12]. Furthermore, the DWC has reduced energy requirements since it is thermodynamically equivalent to the Petlyuk sequence. Dynamic studies have also been developed [13–15], and it has been reported that the DWC shows, in general, good control properties. Other indirect benefits include the fact that a DWC requires less plot area, shorter piping, and less electrical runs; also, a smaller flare system is necessary because of the lower heat input and a smaller fire-case surface [16]. DWC are already used in different processes by many worldwide operating companies, such as BASF AG, M.W. Kellog, Sasol, UOP and others [9, 17]. On the other hand, among the main drawbacks that a DWC may present are: the difficulty to manipulate the vapor distribution between the prefractionator and the main column [18], the more pronounced temperature variation between the top and bottom sections, and the require-

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ment of a single operation pressure for the whole system. Also, in order to be thermodynamically equivalent to the Petlyuk column, the DWC must not show heat transfer across the wall; however, this transfer may occur in practical operation. Nevertheless, it has been reported [19, 20] that energy savings may be achieved by isolating parts of the dividing wall, allowing heat transfer only in certain sections of the wall.

Kim [21] has proposed a separation alternative that consists of a column with two dividing walls. This scheme is simulated as a main column with a prefractionator and an attached postfractionator; in some cases, it shows lower energy requirements than the Petlyuk column, because the postfractionator eliminates the mismatch in composition in the interlinking trays of the Petlyuk column. Gómez-Castro et al. [22] presented a design and optimization methodology for the Petlyuk-like system with a postfractionator, using genetic programming. It was found that the scheme with the postfractionator shows higher thermodynamic efficiency and lower energy requirements than the Petlyuk column, when the mixture to separate contains a low concentration of the intermediate component.

The equations involved in the design of Petlyuk-like systems are highly nonlinear, and the optimization problem for these systems is multivariable; thus, the solution with local optimization methods usually converges to local optima. In the last years, an intensive search for accurate global optimization methods has taken place. Stochastic methods are an important, useful kind of global optimization strategies, requiring reasonable computational times to solve optimization problems with multivariable functions. Moreover, they have the capacity to handle ill-structured or unknown structure problems, usually obtaining results in the near surroundings of the global optimum.

Genetic algorithms (GA) are a part of the stochastic optimization methods, proposed originally by Holland [23]. A GA takes Darwin's concepts of evolution and survival of the fittest as basis. Then, the algorithm evolves a group of solutions (initial population) during a certain number of iterations (generations) using three basic operators: selection, crossover, and mutation, as explained by Goldberg [24] or Gen and Cheng [25]. GA are based on a direct search method, making an explicit knowledge of the mathematical model or its derivatives unnecessary. Moreover, when searching for an optimal solution, the algorithm relies on several points. Then, the selection of the initial values has no influence on the final solution. Taking advantage of these characteristics of the GA, Gutiérrez-Antonio and Briones-Ramírez [26] determined sets of optimal solutions which together form a Pareto front, for the design of Petlyuk columns, obtaining a number of optimal designs instead of a unique solution.

An important design characteristic of the DWC is its diameter. Considering that the shell of the DWC will support the total vapor flow, which corresponds to the side and main columns of the Petlyuk system, special care must be taken when it is dimensioned: The shell must be designed so that it can support the total vapor flow across it, with an appropriate pressure drop. A sizing methodology has been proposed by Premkumar and Rangaiah [27] for the dividing wall column, but no similar method exists for multiple DWC.

In this paper, an adaptation for the sizing methodology of Premkumar and Rangaiah [27] for DWC is proposed. The analyzed system is a double DWC (DDWC) (Fig. 1). The thermodynamically equivalent system (Petlyuk column with postfractionator) is designed using a multi-objective GA with restrictions; this optimization strategy is coupled to the process simulator Aspen Plus™ for the evaluation of objective and constraints functions. To speed up the convergence of the optimization algorithm, the use of artificial neuronal networks (ANN) is considered. Thus, the optimization tool offers the advantage of using the rigorous simulation model in its calculations (no simplifications are required) to obtain the Pareto front of optimal solutions in a relatively short computing time. Two different mixtures with variable feed composition were studied. In general, the design and optimization method shows robustness, and it allows obtaining an adequate set of optimal designs for complex distillation sequences. Furthermore, the sizing method appears to be adequate for multiple dividing wall systems, and, according to the results, the required dimensions of the column for one or two dividing walls are quite similar when the designs are optimal, and thus, the separation costs are dominated by the costs of the utilities.

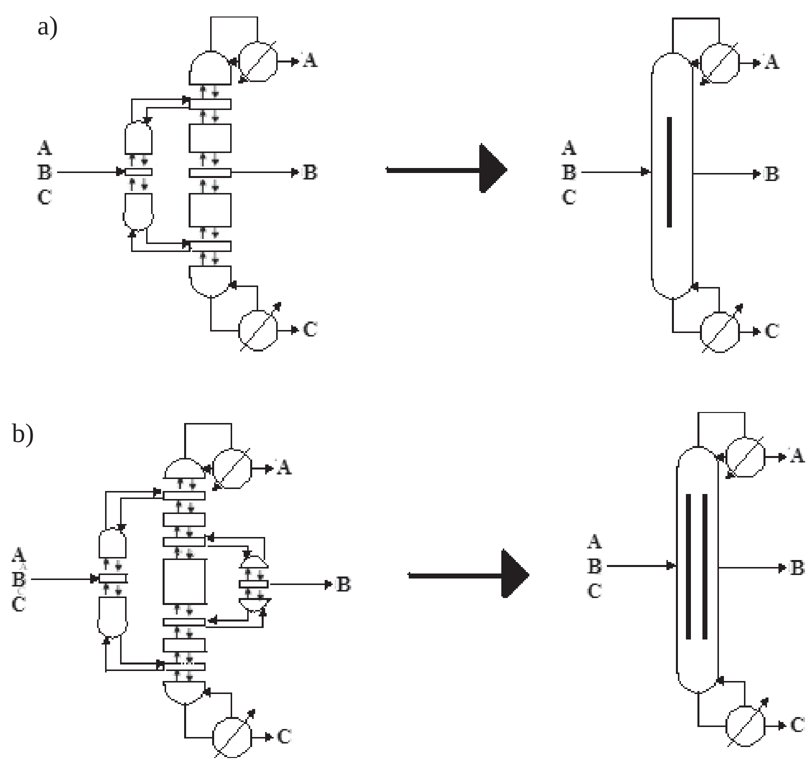

Figure 1. (a) Petlyuk column and DWC, (b) Petlyuk-with-postfractionator system and DDWC.

2 Stochastic Multi-Objective Optimization Strategy

In terms of multi-objective optimization, when a minimization takes place and the algorithm reaches a point where there is no feasible vector that can decrease the value of an objective without simultaneously increasing the value of another objective, it is said that this point in the search space is a Pareto optimum. For distillation columns, the Pareto front represents all optimal designs, from the minimum number of stages to the minimum reflux ratio. The adequate design shall be chosen by selection of a point along the Pareto front.

In the optimization problem of the Petlyuk column with postfractionator sequence, we have to minimize simultaneously the heat duty, Q, and the number of stages, N_{i}, in the prefractionator, the main column and the postfractionator, subject to meet the required recoveries or purities in each product stream. This minimization can be formulated as:

$$\begin{aligned}&\mathrm{Min}(Q, N_{\mathrm{i}}) = f(Q, R, N_{\mathrm{i}}, N_{\mathrm{j}}, N_{\mathrm{s}}, N_{\mathrm{F}}, F_{\mathrm{j}})\\&\mathrm{st}\\&\vec{y}_{\mathrm{k}} \geq \vec{x}_{\mathrm{k}}\end{aligned} \quad (1)$$

where R is the reflux ratio, N_{i} is the total number of stages of the column i, N_{j} is the stage number of the interconnection flow j, N_{s} is the side stream stage, N_{F} is the feed stage number in the prefractionator, F_{j} is the interconnection flow j, and $\vec{x}_{\mathrm{k}}$ and $\vec{y}_{\mathrm{k}}$ are the vectors of required and obtained purities or recoveries, respectively. Eq. (1) represents the general optimization problem for DWC; thus, it may be applied for a DWC or a DDWC, depending on the number of columns, i. As can be noted, in the optimization problem, four variables in competition are considered for optimization: the heat duty of the sequence and the number of stages in the main column, the prefractionator and the postfractionator.

For the described minimization problem, the optimization methodology is required to find values for the design variables, allowing a design where the energy requirements and the number of stages in each column are simultaneously optimized. In this approach, the implemented multi-objective algorithm is based on the NSGA-II [28], and constraints are handled using a modification of the work of Coello [29]. The link to Aspen Plus allows having optimal designs using rigorous simulations; however, 95 % of the total time of the optimization procedure is employed in performing these simulations. Due to this, we use ANN to speed up a multi-objective GA with constraints, based on the work of Gutiérrez-Antonio and Briones-Ramírez [30]. The ANN create approximated functions for objective and constraints, which are used to evaluate the individuals of the population. In this way, the original objective and constraint functions are used just every m generations, and the approximated functions in the rest of them, decreasing the total computational time. This allows reaching the Pareto front very quickly. Fig. 2 shows a block diagram for the evolutionary strategy coupled to the ANN.

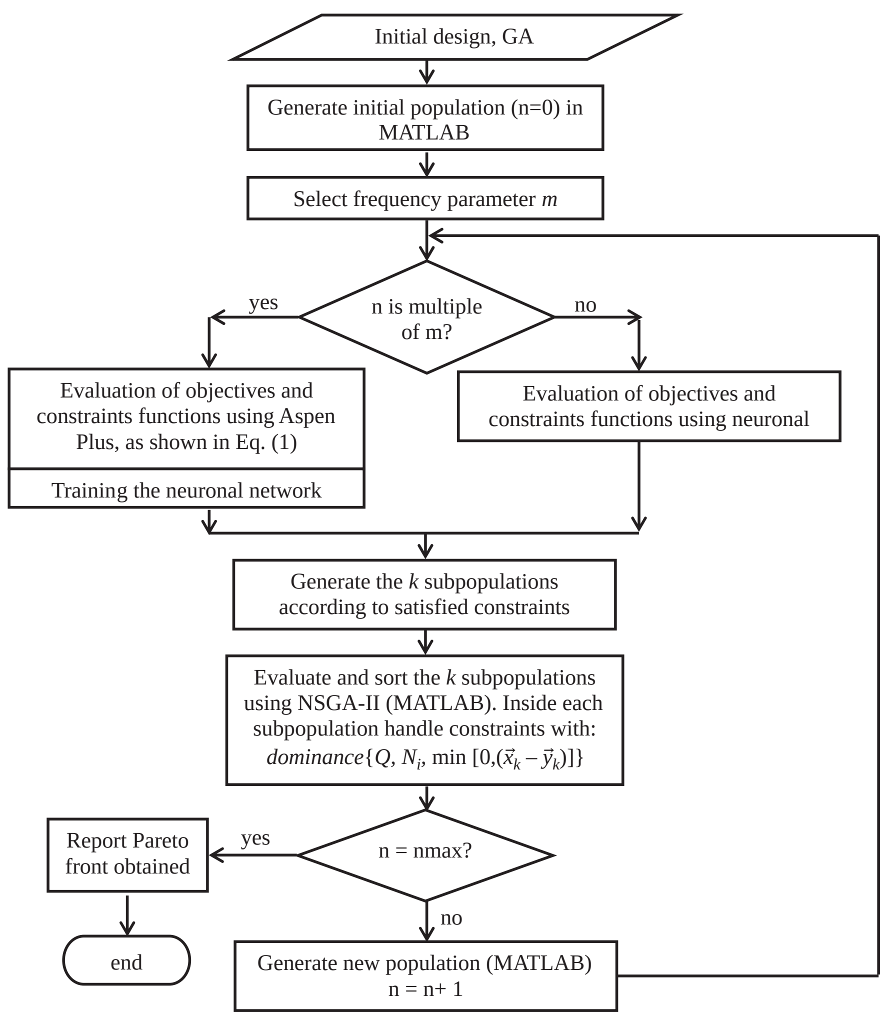

Figure 2. Block diagram for the multi-objective GA with neuronal networks.

3 Sizing of the DWC

Once the optimal design is obtained, an indispensable parameter is the diameter of the column. Premkumar and Rangaiah [27] presented a strategy for columns with a single dividing wall. This method is adapted to calculate the diameter of the DDWC. The first consideration to be taken into account is that the diameter of the column must be large enough to support the vapor and liquid flowing across it. In the case of the DDWC, those flow rates must correspond to the three columns, prefractionator, main column and postfractionator, of the Petlyuk-with-postfractionator system, with the vapor flow being the most important in terms of pressure drop. Taking as a basis the distribution of vapor flow for the DWC established by Premkumar and Rangaiah [27], a distribution of vapor flow for the DDWC is proposed here, as shown in Fig. 3. The flooding condition in the column determines the maximum vapor velocity and, consequently, the diameter of the column. According to Premkumar and Rangaiah [27], the maximum vapor velocity, or flooding vapor velocity, is calculated by:

$$V_{\max} = K_1 \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \tag{2}$$

As proposed by Premkumar and Rangaiah [27], K_1 is taken as 0.07 m s^{-1} for sieve trays, and the operation vapor velocity is considered to be 80 % of the flooding vapor velocity. Thus:

$$V_{\text{act}} = 0.8 V_{\max} \tag{3}$$

Finally, the tray diameter is calculated by

$$D = \sqrt{\frac{4G}{\pi \rho_V V_{\text{act}}}} \tag{4}$$

In Eq. (4), D is the diameter of the tray (m), G is the total vapor flow rate (kg s^{-1}) entering the tray, and ρ_V is the vapor density (kg m^{-3}). The diameter of the column shall equal the diameter of the larger tray, ensuring an adequate distribution of the vapor flow along the column.

4 Cases of Study

Two different feed compositions have been considered in this study. Each composition corresponds to mixtures with different ease of separation index (ESI = α_{AB}/α_{BC}) values, as defined by Tedder and Rudd [2]. The mixtures under analysis are described in Tab. 1. Mixture M1 corresponds to an almost ideal hydrocarbon blend; thus, the Chao-Seader model is good enough to predict the vapor-liquid equilibrium. Mixture M2 is a complex mixture; thus, the NRTL-RK thermodynamic model was used to simulate the liquid-vapor equilibrium. The feed flow rate for M1 was 45.35 kmol h^{-1} and for M2 100 kmol h^{-1}. The required molar purities for M1 are 98.7 % of *n*-pentane, 98 % of *n*-hexane and 98.6 % of *n*-heptane, while for M2 the desired molar purities are 98.6 % of methyl formate, 99.97 % of methanol and 98.3 % of *n*-butanol. The design pressure for each separation was chosen to ensure the use of cooling water in the condensers.

Table 1. Mixtures analyzed.

Mixture	Components	Feed composition (mole fraction)
M1	*n*-pentane, *n*-hexane, *n*-heptane	0.40, 0.20, 0.40
M2	methyl formate, methanol, *n*-butanol	0.06, 0.913, 0.027

The parameters of the stochastic strategy were selected as 50 generations of 1000 individuals each, while the parameter m is fixed as 5; these parameters were obtained from a tuning process. The DWC and DDWC are simulated in the Radfrac module of Aspen Plus.

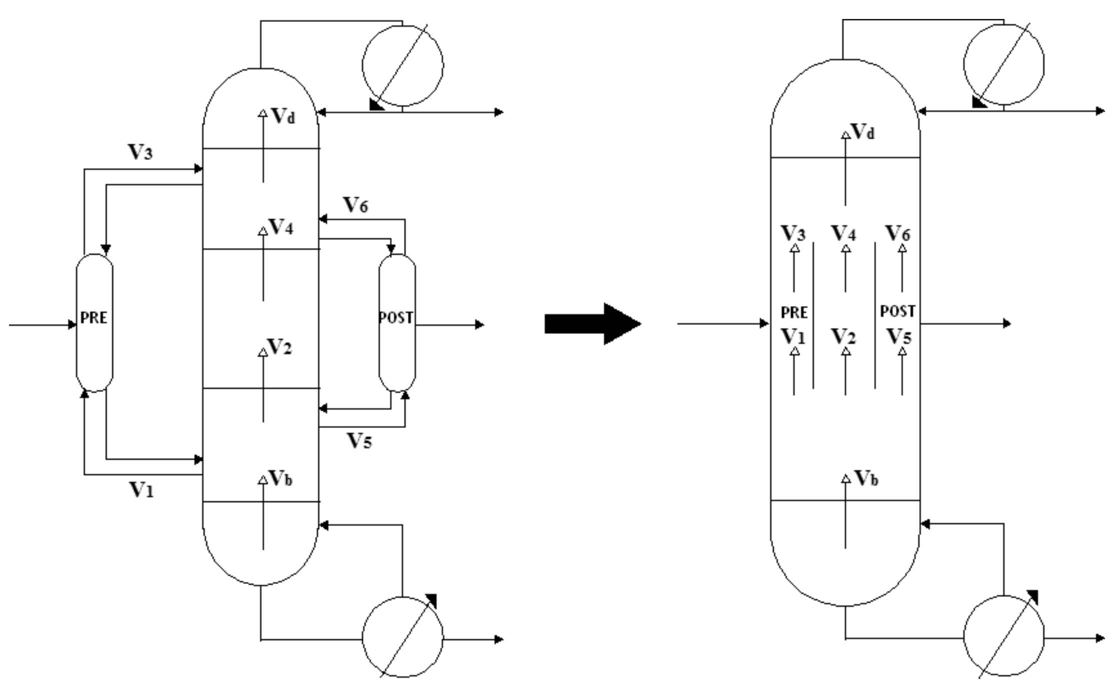

Figure 3. Vapor flow distribution for the DDWC.

5 Results and Discussion

In this section, the results from the design and optimization of the columns will be first discussed. Then, sizing results will be shown and these results will be complemented with a cost analysis. For comparison purposes, the results will be shown for both systems, DWC and DDWC. In Fig. 4, the Pareto fronts obtained from the multi-objective GA for the DWC and the DDWC are presented. It can be seen that both the DWC and the DDWC show a similar performance in terms of the reboiler duty for mixture M1, but this does not occur in the case of mixture M2. From each Pareto front, ten designs have been selected to be analyzed.

The distribution of the stages for these designs is presented in Tabs. 2 and 3 for mixtures M1 and M2, respectively. N_{MC} is the number of stages in the main column, N_{PRE} is the number of stages in the prefractionator, and N_{POST} is the number of stages in the postfractionator. Of course, once a DDWC is considered, N_{PRE} will be the number of stages of the main column occupied by the first dividing wall, and N_{POST} will be the number of stages of the main column occupied by the second dividing wall. For the DWC, N_{PRE} is the number of stages of the main column occupied by the single dividing wall. It was found that, for mixture M1, there is an occupation of about 20–30 % of the main column for the DWC, while for the DDWC there is an occupation of 15–30 % for both dividing walls in the majority of cases. This variation in the distribution of the two dividing walls may be attributed to the ESI of the mixture, which is only slightly higher than 1. Thus, the easiness of separation of the pair *n*-pentane/*n*-hexane is close to the corresponding one of the pair *n*-hexane/*n*-heptane. Moreover, the total molar flow rates of the interlinking flows enter-

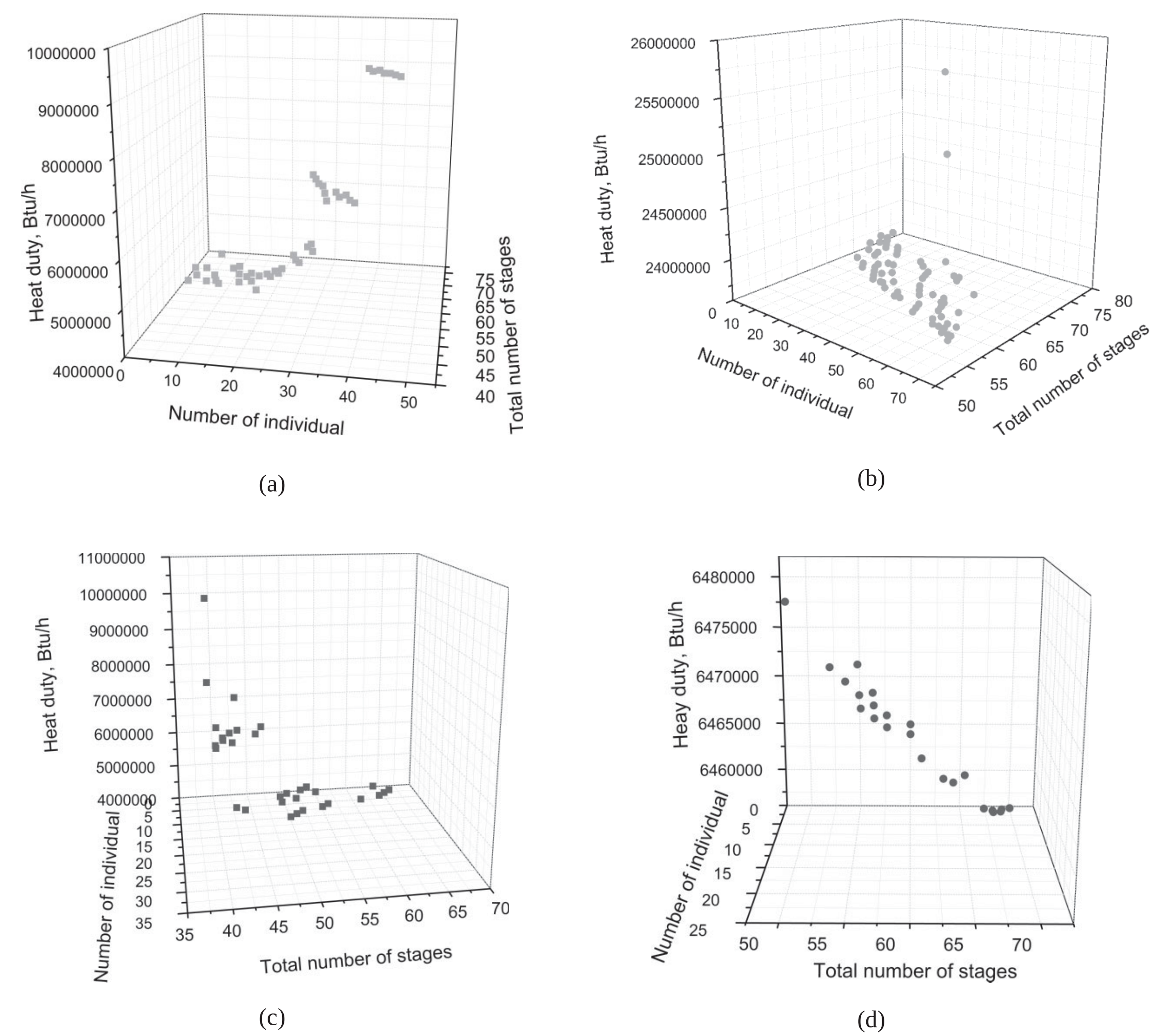

Figure 4. Pareto fronts for the DDWC. (a) Mixture M1, (b) mixture M2.

ing the prefractionator and the postfractionator are quite similar; thus, when designing the prefractionator and the postfractionator, there are different configuration alternatives that can achieve the desired purity. On the other hand, for mixture M2, the second dividing wall tends to occupy a higher number of stages than the first dividing wall. Moreover, the second dividing wall of the DDWC covers a higher number of stages than the unique dividing wall of the DWC. This can be explained in terms of the flow rates. First of all, the mixture consists of a high proportion of methanol, with a low content of methyl formate and an even lower content of *n*-butanol. Furthermore, the separation taking place in the postfractionator is not an easy task, because a high purity of methanol is required, and the molar flow rates of the interlinking flows entering the postfractionatior are quite higher than those entering the prefractionator; thus, a higher number of stages is required to eliminate the impurities in the postfractionator. The energy requirements for the selected designs of the DWC and DDWC are shown in Tab. 4. It can be seen that, for mixture M1, the DDWC shows lower energy requirements than the DWC. On the other hand, for mixture M2, the DWC presents lower heat duty. Thus, the DDWC has potentially low energy requirements for mixtures with a low content of the middle-boiling component in the feed. For mixtures with a high content of such a component, the DWC is, in terms of energy requirements, the best alternative between the two systems under analysis.

Table 2. Distribution of stages of ten selected designs from the Pareto front, M1.

	Petlyuk column									
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
N_{MC}	51	40	54	54	54	51	45	45	41	40
N_{PRE}	13	15	12	11	10	10	11	10	11	11
	Petlyuk with postfractionator									
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
N_{MC}	45	42	45	43	51	42	45	42	42	44
N_{PRE}	13	9	10	17	8	8	9	7	9	16
N_{POST}	10	11	9	7	14	12	10	13	10	7

Table 3. Distribution of stages of ten selected designs from the Pareto front, M2.

	Petlyuk column									
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
N_{MC}	59	59	58	58	57	57	54	53	53	51
N_{PRE}	11	10	11	10	11	10	10	12	10	10
	Petlyuk with postfractionator									
	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
N_{MC}	57	56	54	57	53	57	51	57	49	56
N_{PRE}	6	9	6	7	8	6	7	6	6	6
N_{POST}	12	12	12	11	12	11	12	10	12	10

Table 4. Energy requirements for the analyzed systems (kJ h^{-1}).

	DWC	DDWC
M1	4 310 507.82	2 657 889.06
M2	4 301 272.92	5 216 496.47

Sizing was performed for the first case appearing on the Pareto front (S1) for DWC and DDWC. The results of such calculations are shown in Tab. 5. For comparison purposes, the diameter of the optimal design selected and the diameter for the initial, non-optimized designs are shown. Initial designs for the DWC have been obtained using the stage rearrangement methodology proposed by Hernandez and Jimenez [5], obtaining the number of stages and the location of the feed stages for the Petlyuk column based on a three-column conventional sequence. The designs for the conventional sequence were calculated by using the Winn-Underwood-Gilliland method. Values for the interlinking streams are first postulated and then adjusted to reach the design specifications. On the other hand, for the initial designs of the DDWC, the number of stages in the main column and the prefractionator are considered as equal to those of the DWC, and the location of the interlinking streams between the prefractionator and the main column are also taken as equal to those of the DWC. In the case of the postfractionator, the number of stages is postulated, with the restriction that the number of stages in the postfractionator must be smaller than the number of stages in the prefractionator. The location of the interlinking stages is also postulated, but a restriction is imposed for which the postfractionator must be located in the same region corresponding to the prefractionator. As for the DWC, interlinking flow rates are postulated and then adjusted to achieve the desired purities. Due to all the postulated values, the initial designs are expected to be located in a region far from the optimum. The diameter shown in Tab. 5 corresponds to the higher tray diameter calculated, since the diameter does not appear to vary considerably for the different trays of the columns. It was observed that the use of a DDWC may enhance the vapor distribution in the column, and this may partly explain the reduction in energy consumption for the purification of mixture M1. As can be expected, an optimized design not only reduces the energy requirements but also allows a better vapor flow distribution, which results in lower required diameters. Furthermore, the difference between the diameter of the DWC and the

DDWC is not greater than 0.15 m. Thus, it could be expected that the difference between the construction costs for both schemes is small, and the most convenient system will be defined by the costs of the utilities. To prove this affirmation, cost estimations were made. To estimate the costs for the DWC, Guthrie's method was used [31]. The height of the columns was evaluated with an equation proposed by Heaven [32]. Nevertheless, some additional assumptions must be made to take into account the characteristics of the DWC. The cost of the vessel was considered to be 20 % higher than the cost corresponding to a conventional system with the same dimensions, and the cost of the trays where dividing walls must be located is taken as 30 % higher than the cost of standard sieve trays [33]. The results for the cost calculations are shown in Tab. 6. Costs for equipment were annualized considering a recovery time for investment of 5 years. In Tab. 6, costs are shown for equipment, utilities and the TAC. It can be seen that the utility cost makes the most important contribution to the TAC, for all the analyzed cases. Thus, for mixture M1, the DDWC shows lower TAC since it allows a considerable reduction on the energy requirements for the separation. On the other hand, for mixture M2, the DWC allows a lower heat duty and, consequently, lower TAC.

Table 5. Diameter calculation results.

	DWC (optimum)	DWC (initial)	DDWC (optimum)	DDWC (initial)
M1	1.02	2.15	0.94	2.05
M2	0.95	1.91	1.08	1.67

Table 6. Total annual cost estimations (US$ a^{-1}).

	DWC			DDWC		
	Equipment	Utilities	TAC	Equipment	Utilities	TAC
M1	75 571	1 098 594	1 174 165	65 200	658 324	723 524
M2	84 232	1 118 658	1 202 890	85 341	1 412 423	1 497 764

6 Conclusions

A design and optimization methodology for dividing wall distillation systems was proposed. This method is based on a multiobjective GA with constraints coupled to the Aspen Plus simulator. A Petlyuk-like system with a postfractionator was analyzed. Based on the results obtained for the Petlyuk-with-postfractionator system, a sizing strategy for the thermodynamically equivalent DDWC is applied. The GA used has shown to be an adequate and relatively simple tool for the design and optimization of complex systems, when an appropriate selection of the genetic parameters is performed. The results show that, for a mixture with low composition of the middle-boiling component, the Petlyuk-with-postfractionator system may show savings of up to 38 % on energy consumption compared to the Petlyuk column, when a good design and optimization method is used. On the other hand, when the mixture contains a high composition of the middle-boiling component, the Petlyuk column has a better performance in terms of the energy requirements, with energy savings of at least 17 % relative to the Petlyuk-with-postfractionator system. Furthermore, it appears to be clear that, for this kind of mixture, even little changes in the structure of the Petlyuk-with-postfractionator system may considerably change the thermal duty, possibly affecting the dynamic performance of the column.

The considered sizing methodology for the DDWC is based on the internal flows across the column. According to the results, the use of one or two dividing walls does not considerably affect the required diameter of the column, with only small variations. This may be explained considering that the total vapor flowing across the column is almost the same for both columns; thus, the methodology used for sizing a column with a single dividing wall may be successfully applied even if a higher number of dividing walls is used. In the case of mixture M1, the DWC requires a slightly higher diameter than the DDWC, while the opposite occurs in the case of mixture M2. As a consequence, when estimating TAC, it has been found that the TAC for the DDWC are lower than those corresponding to the DWC when the middle-boiling component has a low content in the feed stream. The opposite occurs when a mixture with a high content of the middle-boiling component in the feed stream is separated. Thus, the choice on using a single or multiple dividing walls column may depend firstly on the feed composition of the mixture to be separated, because the feed composition has an important influence on the reductions on energy requirements, and consequently on the TAC, for the DDWC. According to the results, the purification of a mixture with a low content of the middle-boiling component using a DDWC allows obtaining lower heat duty and TAC than that corresponding to the same separation with a DWC.

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Symbols used

D	[m]	diameter of the column
G	[kg s^{-1}]	vapor flow rate
V_{max}	[m s^{-1}]	flooding vapor velocity
V_{act}	[m s^{-1}]	actual vapor velocity

Greek symbols

ρ_L	[kg m^{-3}]	density of the liquid phase
ρ_V	[kg m^{-3}]	density of the vapor phase

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