21st European Symposium on Computer Aided Process Engineering – ESCAPE 21
E.N.. Pistikopoulos, M.C. Georgiadis and A.C. Kokossis (Editors)

Optimal design of multiple dividing wall columns based on genetic programming

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Abstract

In this work, two schemes are analyzed for the reduction on energy consumptions for ternary distillation: a Petlyuk column, PC, and a Petlyuk with postfractionator system, PCP. To perform the optimal design of the analyzed systems, the use of multiobjective genetic algorithms has been considered. Moreover, a strategy for diameter calculation is proposed for the dividing wall column, DWC, and double dividing wall column, DDWC, which is based on their distribution of internal flows. Results show that genetic algorithm tool allows obtaining optimal designs for the PC and PCP systems, with low energy consumptions. Furthermore, the design strategy for the DWC and DDWC shows that the physical structure required for one or two dividing walls is quite similar; thereby, it appears to be an adequate method for the sizing of the dividing wall systems.

Keywords: Multiple dividing wall columns, stochastic optimization, columns sizing.

1. Introduction

Thermally coupled distillation sequences are a good option to reduce energy consumption in the separation of fluid mixtures. One of the more important thermally coupled schemes is the Petlyuk column, which may reduce energy requirements up to 30% in comparison to conventional sequences [1]. An alternative system, recently analyzed, consists on a Petlyuk system with an additional column attached, known as postfractionator; in some cases, this system can achieve even lower heat duties than the Petlyuk column [2]. Because of mechanical issues, a thermodynamically equivalent system known as the dividing wall column is used instead of the Petlyuk column; for the Petlyuk column with postfractionator it has been proposed that its equivalent could be a double dividing wall column [3]. A dividing wall column consists in a shell, in which a metallic wall is inserted; thus an appropriate diameter must be used to support the maximum vapor flow rate, allowing a proper pressure drop along the column and avoiding flooding. A strategy to calculate the diameter of the DWC has been recently proposed [4], based on the vapor flow rate distribution on the column; nevertheless, there is no such methodology for DDWC. Therefore, in this work an extension of the methodology for the DWC is proposed to obtain proper diameter calculations for the DDWC. To obtain low-energy designs for the dividing wall systems, a multiobjective genetic algorithm has been used to find the Pareto front of optimal designs for the DWC and DDWC. The optimal designs obtained offer a good distribution of the vapor flows, which allows requiring trays with a lower diameter.

2. Design and optimization tool: multi objective genetic algorithm

The design and optimization of the analyzed systems have been performed by using a multi objective genetic algorithm with constraints, coupled to the process simulator Aspen Plus. Due to the characteristics of the search space, conventional derivative-based optimization methodologies may present considerable difficulties finding a solution near to global optimum, while stochastic optimization algorithms are robust and efficient tools for solving such optimization problems. When a multiobjective optimization is considered, the set of solutions found by the genetic algorithm is known as the Pareto front. In the case of Petlyuk-like distillation columns, the multiobjective optimization considers the simultaneous minimization of the heat duty of the sequence, and the number of stages in each column of the scheme. The minimization problem is formulated as:

$$\begin{aligned}&\min(Q, N_i) = f\left(Q, R, N_i, N_j, N_s, N_F, F_j\right)\\&s.t.\\&\overrightarrow{y_k} \geq \overrightarrow{x_k}\end{aligned} \quad (1)$$

Where R is the reflux ratio, N_i is the total number of stages in the column i, N_j is the stage number of the interlinking flow j, N_s is the side stream stage, N_F is the feed stage number in the prefractionator, F_j is the interlinking flow, and $\overrightarrow{x_k}$ and $\overrightarrow{y_k}$ are the vector of required and obtained purities or recoveries. During the optimization process the most consuming time activity is the evaluation in Aspen Plus of the objectives and constraints. For that reason, we speed up the multiobjective strategy using neuronal networks, decreasing in at least 50% the computational time [6].

3. Calculation of the diameter of the dividing wall columns

For the determination of the diameters of these systems, the strategy presented by Premkumar and Rangaiah [4] for the DWC has been extended for the DDWC. For a single tray:

$$D = (4G/0.8\pi\rho_V V_{max})^{1/2} \quad (2)$$

In Eq. 2, D is the diameter of the tray (m), G is the total vapor flow rate (kg/s), and ρ_V is the vapor density (kg/m^3). It has been considered that the actual vapor velocity corresponds to the 80% of the maximum vapor velocity, V_{max}. The equivalencies for the vapor flows for the DDWC are shown in Figure 1.

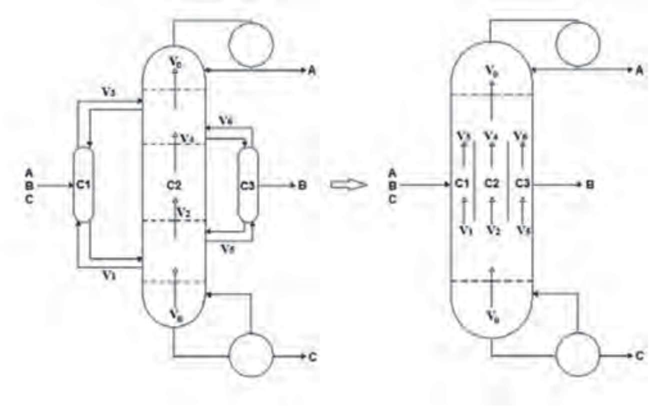

Figure 1. Vapor flow distribution for the double dividing wall column.

The two dividing walls in the DDWC are represented in the PCP system by the prefractionator and the postfractionator. Thus, the trays on the DDWC must be designed to support the vapor flowing not only through the main column, C2, but also the vapor on the side columns, C1 and C3. A similar approach is considered for the DWC, where only the columns C1 and C2 exist. The diameter of the DWC and DDWC is taken as equal to that of the larger tray, since it has the higher vapor rate flowing across it. V_{max} is the flooding vapor velocity, and is given by:

$$V_{max} = K_1(\rho_L - \rho_V/\rho_V)^{1/2} \quad (3)$$

K_1 has been considered as 0.07 m/s, as proposed by Premkumar and Rangaiah for the DWC using Sieve trays [4].

4. Case of study

The analyzed mixtures are shown in Table 1. It can be seen that the mixture M1 has a low molar feed composition of the middle-boiling component, n-hexane, while mixture M2 has a high composition of the middle-boiling component, methanol, in the feed stream. Pareto fronts of both Petlyuk-like schemes have been generated with the multiobjective genetic algorithm; the parameters of this optimization were 50 generations of 1000 individuals each one. From the Pareto front, 10 optimal designs were selected and their simulations were analyzed with more detail.

Table 1. Analyzed mixtures

Mixture	Component	Feed Composition	Feed Flowrate, kmol/h	Purity
M1	n-pentane	0.40	18.14	98.70%
	n-hexane	0.20	9.07	98.00%
	n-heptane	0.40	18.14	98.60%
M2	methyl formate	0.06	6.0	98.60%
	methanol	0.913	91.3	99.97%
	n-butanol	0.027	2.7	98.30%

5. Results

Since this work has been developed to observe the performance of the DDWC, In Figure 2 the Pareto fronts for the DDWC are shown.

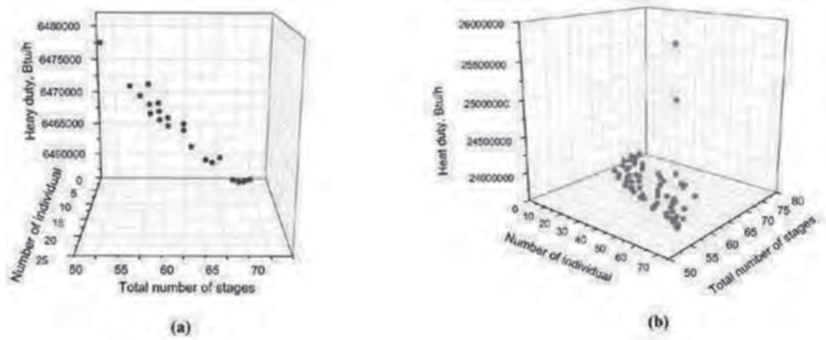

Figure 2. Pareto fronts (a) M1, (b) M2

For the mixture M1 the energy consumption for the DDWC has been observed to be lower or similar than for the DWC. For mixture M2, in most cases the DWC shows lower energy consumption, and even small changes in the structure of the DDWC may have a great impact on the heat duty of the system, as can be seen in Table 2, where the distribution of stages on the columns in shown.

Table 2. Distribution of stages, M2

Case	1	2	3	4	5	6	7	8	9	10
$N_{MC,DWC}$	59	59	58	58	57	57	54	53	53	51
$N_{PRE,DWC}$	11	10	11	10	11	10	10	12	10	10
$N_{MC,DDWC}$	57	56	54	57	53	57	51	57	49	56
$N_{PRE,DDWC}$	6	9	6	7	8	6	7	6	6	6
$N_{POST,DDWC}$	12	12	12	11	12	11	12	10	12	10

In Table 3 calculated diameters for the respective lowest energy consumption cases are shown. To compare, calculated diameters for the initial, non-optimized designs are shown. Those initial designs have been obtained by short-cut methods. It is clear that the diameter required for a single and a double dividing wall column is not quite different. It also can be seen that the diameter for the optimal designs results lower than the required for the non-optimal designs. Thus, the design and optimization methodology presented allows a better vapor flow distribution and lower diameters, which will have a direct impact on equipment costs.

Table 3. Calculated diameters (m)

Mixture	DWC, opt	DWC, init	DDWC, opt	DDWC, init
M1	1.02	2.15	0.94	2.05
M2	0.95	1.91	1.08	1.67

6. Conclusions

In this work a design and optimization strategy based on evolutionary techniques has been presented. The multiobjective genetic algorithm allows obtaining a number of optimal solutions to the design and optimization problem. It has been found that a good design of the DDWC presents lower energy requirements than the DWC for mixtures, where the middle-boiling component appears in a low concentration on the feed stream. On the other hand, when the composition of the middle-boiling component on the feed is high, the DWC is the best alternative, since even small changes in the structure of the DDWC may increase considerably the energy requirements. According to the diameter calculations, the diameter required for a dividing wall column appears to be quite similar when using one or two dividing walls, thus it is expected that the shell construction costs are not different for both cases. Furthermore, the optimization methodology allows obtaining designs with a good vapor flow distribution, thus requiring lower diameters for the shell of the dividing wall systems. Those designs are compared in terms of energy, trays and diameter for the same separation, and interesting trends have been obtained.

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