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OPTIMAL DESIGN METHODOLOGY FOR DIVIDING WALL COLUMNS

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Abstract
The dividing wall column, DWC, is a thermally coupled sequence that can perform the separation of fluid mixtures with reduced energy consumption, but also decreasing the capital costs associated. Several authors have developed design procedures for this kind of sequence, using short methodologies or optimization strategies. The use of short procedures is easy and fast, but, in the most of the cases, the resulting design is not optimal. On the other hand, the use of optimization procedures allow obtaining optimal designs, but time and complexity required are elevated. In this work, we propose an optimal and short design methodology for DWC. First, we use a multiobjective genetic algorithm with constraints, coupled to Aspen Plus, to obtain Pareto fronts of DWC for different mixtures, feed compositions and recoveries. The analysis of the Pareto fronts brings useful information about the flows and composition of the interconnection flows, key variables in this methodology, which are incorporated in a short method that generates optimal designs with less computational resources.

Keywords: optimal design, dividing wall column, short procedure

1. Introduction

Thermally coupled distillation sequences are the most promising option to separate fluid mixtures with reduced energy consumption. There are several thermally coupled configurations, within which the Petlyuk column brings the major reduction in energy consumption[1-3]. Usually, the physical implementation of the Petlyuk column is performed in a single shell, as a dividing wall column, DWC. The DWC reduces operating costs in 35%, investment costs in 25%, and also the requirements of space in 40%, in comparison with a conventional column system[4]. Hence, there are better prospects of DWC in the near future, and it might become a standard distillation configuration in chemical process industries in the next 50 years[4]. Several authors have developed design procedures for the DWC, using the short procedure of Fenske-Underwood-Gilliland[3, 5-6], or optimization procedures[7-12].

The principal advantage of the procedures[3, 5-6] based on Fenske-Underwood-Gilliland is their simplicity, since just algebraic equations are considered. Thereby, its application is very easy and quickly we can obtain a design of the DWC. The principal disadvantage is that, like the Fenske-Underwood-Gilliland method, these methods are good for ideal mixtures or nearly ideals; additionally, it is well known that the correlation of Gilliland differs considerably for some feeds or recoveries cases[13]. Also, in the particular case of the DWC, initial values for the interconnection streams, as flow as compositions, are not given; since estimate the distribution of the components in the prefractionator is not an easy task, and it depends of the nature of mixture, feed composition and desired recoveries[12].

On the other hand, the optimization procedures[7-12] guides the search to find the optimal design (considering one or multiple objectives) using, principally, mathematical programming or stochastic strategies. The optimization of a distillation column, even the simpler, is a mixed integer non linear problem with constraints. The high complexity of the problem has originated that the optimization algorithms, in the most of the cases, used reduced models. The fact is that the implementation of any of these strategies is not an easy task, since deep knowledge of mathematical programming or stochastic strategies, along with considerable computational resources are required.

From the briefly descriptions made before, it would be desirable to have the best of both procedures; in other words, having a short design methodology, easy to implement, that also brings the optimal design of the DWC. The contribution of this work is focus in that direction. The Figure 1 shows the dividing wall distillation column, which is thermodynamically equivalent to the Petlyuk configuration, and it also can be represented as a sequence of three disengaged distillation columns. If we observe carefully the sequence of three disengaged distillation columns along with the DWC, Figure 1, it is clear that the interconnection flows are the key in the design of the DWC.

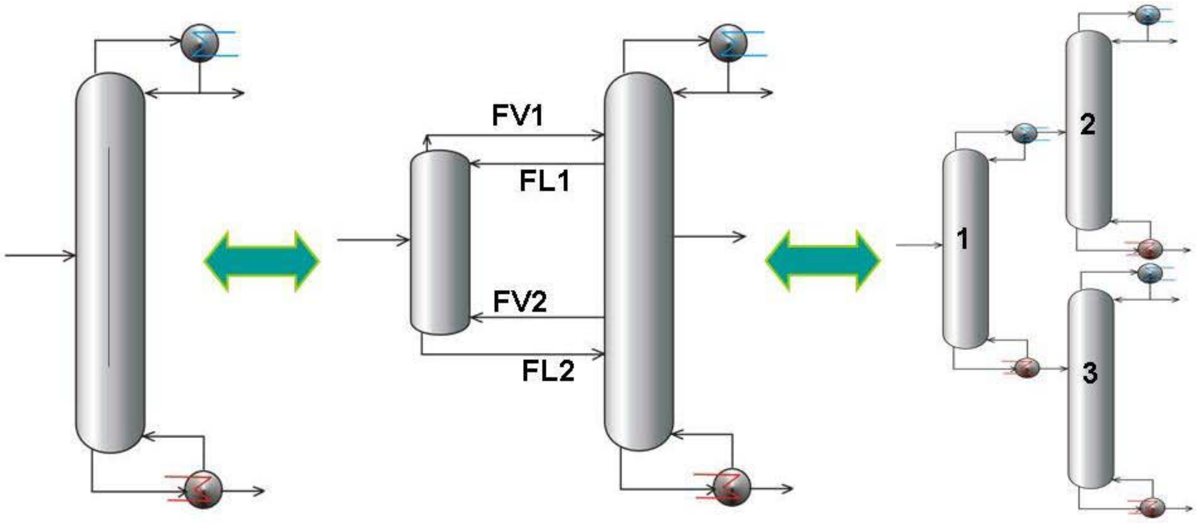

Figure 1. Dividing wall column and its representation as a sequence of three disengaged columns

In the sequence of three disengaged columns, columns 2 and 3 can be also considered as side-stream columns, since they have one feed stream and one product stream that returns to the first column. In column 2 the feed stream is the interconnection flow FV1, while the interconnection flow FL1 is the side-stream product, which returns to the column 1. For analogy, the interconnection flow FL2 is fed to column 3, while the interconnection flow FV2 is a side-stream product that returns to the column 1. Therefore, once we knowing the compositions and flows of two interconnection streams, FL1 and FV2, it is relatively simple to design the three disengaged distillation columns, and, finally, the DWC or the Petlyuk sequence.

On the other hand, from the review of the previous methodologies we have found some clues about the importance of the interconnection streams. For instance, in the work of Hernández and Jiménez[3] a minimization of the interconnection flows is performed in order to get the optimal design for a given structure; similar observations are found in the other methodologies[5-12]. Virtually, the interconnection flows represent not just how much liquid or vapor flows are recycling inside the sequence, but also the compositions gradients present. In this way, the interconnection flows not just determine the performance of the separation, but also help to soften the disturbance in the column[3]. Then, we can affirm that if somehow we know the optimal values for at least two interconnection flows (FL1 and FV2), then we can design an optimal column, applying, for instance, a method based on the minimum composition difference[15].

Now, the values and composition of the interconnection streams depend on the nature of the mixture, feed composition and recoveries of the key components[12]. One option is analyze all available and existing designs of the DWC in order to get the information about the interconnection streams; however, we can not ensure that these designs correspond to global optimum. Another option could be analyze the material balances for several feed compositions and recoveries, but given the wide variety of mixtures this task is consuming time and not efficient. Then, another strategy must be implemented. So, we decided to use a previous contribution[12] to obtain the required data about the interconnection streams; this tool is a multiobjective genetic algorithm with constraints, coupled to Aspen Plus. This algorithm allows having optimal designs, considering the complete model of the distillation units due to its link to Aspen Plus; also, since a Pareto front is generated in just one run, we have a set of optimal designs, from minimum reflux ratio to minimum number of stages, to analyze.

So, in this work we propose a short and optimal design methodology for dividing wall columns. The methodology consider the DWC as a sequence of three disengaged columns: the first one is a single distillation column, while the other two are considered as side-stream distillation columns. The design of these columns is performed with an optimal design methodology[15] based on the concept of minimum composition difference. In order to design the three distillation columns, we use estimations of the composition and flows of the interconnection streams; these estimations were obtained from the analysis of 100 Pareto fronts of seven ternary mixtures, with 4 different feed compositions and three recoveries. Then, the estimations of the interconnection streams variables are considered as a function of the easy separation index[16] of the mixture, their feed composition and the desired recoveries for the key components. The easy separation index is introduced with the aim to consider the nature of the mixture in the estimation. The method is tested with different ternary mixtures, and it is compared with the results of a multiobjective genetic algorithm with constraints[12], linked to Aspen Plus™. Results show that designs obtained with the new procedure are very similar to those obtained through stochastic optimization, but less time and computational resources are required.

2. Methodology

The methodology consider the DWC as a sequence of three disengaged columns: the first one is a single distillation column, while the other two are considered as side-stream distillation columns. The design is performed in three steps; first, the estimation of flows and compositions of the interconnection flows must be calculated, since they are used to design the three columns; second, the column 1, see Figure 1, is designed with the optimal design methodology based on the concept of minimum composition difference[15]. At this point we use the estimations for the interconnection flows resulting from the analysis of the rigorous Pareto fronts. Once that column 1 is designed, then we continue with columns 2 and 3, which are considered as side-stream columns. The use of the optimal methodology based on the concept of minimum composition difference guarantees that the structures of the three columns are optimal, for the interconnection flows considered.

The key step in this methodology is the generation of the estimations for the composition and flows of the interconnection streams. Basically, once we have these estimations, a methodology for single columns can be applied to obtain the complete design. It is important to consider that we are expecting that the estimation of the interconnection flows being optimal or near to the optimal, so the design methodology to define the structure must also to be optimal. Because of this and due to the space limitations we focus our attention in the estimation of the variables of the interconnection flows.

In order to generate the estimations of the values and compositions of the interconnection flows, we calculate Pareto fronts of seven ternary mixtures: pentane-hexane-heptane; propane-butane-pentane; octane-nonane-decane; butane-isobutene-pentane; butane-pentane-isopentane; ethanol-propanol-butanol; and benzene-toluene-xylene. The selected mixtures include ideal, isomers, alcohols and aromatic compounds, with easy separation index equal, greater and minor than the unity. The feed compositions are saturated liquid with four different distribution of components: F1(33/33/34), F2(60/20/20), F3(20/60/20), F4(20/20/60). Also, three recoveries of key components are considered: R1(98%), R2(98.5%), and R3(99%). As parameters for the genetic algorithm, to generate the Pareto fronts for analysis, we selected 40 generations of 600 individuals each one. Using the information of the Pareto fronts, we make an analysis in order to have estimations of the values and compositions of the interconnection streams FL1 and FV2 as function of the easy separation index[16] of the mixture, their feed composition and the desired recoveries for the key components. These estimations are used to design the three disengaged distillation columns, and, finally, the dividing wall column.

3. Case of study

The design method is applied to several ternary mixtures, all of them different from the used to estimate the interconnection flows; due to spaces limitations the results of two of them are presented: isopentane-pentane-hexane (M1), benzene-toluene-ethylbenzene (M2). Feed compositions are F1(33/33/34), F2(40/20/40), for both mixtures; recoveries of key components in each stream of interest are 98% for both mixtures. Thermodynamic model employed is Chao-Seader for liquid mixtures, for liquid phase, while ideality is consider in vapor phase. The feed stream is introduced as saturated liquid. On the other hand, these designs were optimized using a multiobjective genetic algorithm with constraints[12], coupled to Aspen Plus; so, all optimal designs are rigorous. As parameters of the evolutionary strategy, we selected 40 generations of 600 individuals each one.

4. Analysis of results

For all Pareto fronts, generated with seven mixtures, four feed compositions and three recoveries, we perform a simple multivariable lineal regression to estimate the flows of the interconnection streams. We choose this kind of regression since in a previous contribution[12] we found that between the set of optimal designs of the Petlyuk column there were linear relations, in spite of the high non linearity of the problem. The proposed correlation has the following form:

$$z = a + b(ESI) + c(x_{FA}) + d(x_{FB}) \tag{1}$$

Where *z* is the flow of the interconnection stream, FL1 or FV2. The Eq. 1 is function of the easy separation index (ESI) and of the feed composition of the light and intermediate components (X_{FA} and X_{FB}). In this correlation the recoveries are not considered, since they do not have a great influence in the estimation of the variables mentioned before. Table 1 shows the coefficients found for the variables of interest. It is important to mention that the estimation of the interconnection flows is made in lbmol/h, and considering a feed flow of 100 lbmol/h.

Table 1. Coefficient matrix to estimate the flows of the interconnection streams according to Eq. 1

Coefficient	a	b	c	d
FL1	46.9394	5.5266	-15.9174	-16.1425
FV2	102.2032	-16.9448	-14.1832	10.5431

In order to estimate the compositions of the four interconnection flows, we analyze these variables in the optimal designs of all Pareto fronts. We found some tendencies in the compositions of the interconnection flows as a function of the easy separation index, shown in Table 2.

Table 2. Compositions of light (A), intermediate (B) and heavy (C) components of the interconnection flows as a function of the easy separation index

Component	A	B	C	A	B	C	A	B	C
Flow	ESI<1			ESI=1			ESI>1		
FL1 (x)	0.44	0.55	0.01	0.50	0.49	0.01	0.59	0.40	0.01
FV2 (y)	0.03	0.96	0.01	0.01	0.58	0.41	0.01	0.88	0.11
FV1 (y)	0.50	0.48	0.02	0.66	0.33	0.01	0.59	0.40	0.01
FL2 (x)	0.02	0.77	0.21	0.01	0.44	0.55	0.01	0.85	0.14

It is important to mention that in the optimal designs, the values of the interconnection flows FV1 and FV2 are equal; thereby, knowing the estimation for FV2 interconnection flow we also know the value of the FV1 interconnection flow. Also, according to the material balance the interconnection flow FL2 is calculated as function of the feed and FL1 streams:

$$FL2 = FL1 + F \tag{2}$$

In this way, we can make the estimations of the values and compositions of all interconnection streams; with this information, a design procedure can be applied to obtain the sequence of three disengaged distillation columns. As an additional observation, we note that the convergence of the simulation of the sequences is faster when the estimated compositions, Table 2, and flows, Eq. 1 and Table 1, are used as initial estimations of the compositions of the interconnection flows.

Now, we apply the Eq. 1 to calculate the flows of the interconnection streams FL1 and FV2, along with the estimated compositions for all interconnection streams in Table 2 to the study cases defined in the previous section. The Table 3 shows the estimation of flows and compositions for the interconnection flows for the mixture M1. It is worth of mention that the optimal designs for the study cases were reported before[12], and they were not consider in the data to generate the regression.

Table 3. Flows and compositions of the interconnection flows, mixture M1

Case	ESI=0.47	FL1	FV2	FL1 X_A	FL1 X_B	FV2 Y_A	FV2 Y_B	FV1 Y_A	FV1 Y_B	FL2 X_A	FL2 X_B
M1F1	This work	38.95	93.03	0.440	0.550	0.030	0.960	0.500	0.480	0.020	0.770
	Evolutionary	54.34	114.08	0.444	0.551	0.024	0.967	0.497	0.479	0.018	0.769
M1F2	This work	39.94	90.67	0.440	0.550	0.030	0.960	0.500	0.480	0.020	0.770
	Evolutionary	32.72	97.51	0.420	0.500	0.032	0.945	0.487	0.491	0.022	0.781

From the Table 2 we can observe that the estimation of the flow of the interconnection streams is good enough, consider that just the easy separation index and the feed composition is used. On the other hand, we observe a really good estimation of the compositions of the interconnections streams, in spite of this mixture was not considered in those selected to generate the Pareto fronts. Basically, the interconnection flows FL1 and FV1 are pseudo binaries (light and intermediate), while interconnection flows FV2 and FL2 have the intermediate component in major proportion. This observation applies to mixture with an easy separation index minor than the 1.

The Table 4 shows the estimation of flows and compositions for the interconnection flows for the mixture M2. It is worth of mention that the optimal designs for the study cases were reported before[12], and they were not consider in the data to generate the regression.

Table 4. Flows and compositions of the interconnection flows, mixture M2

Case	ESI=1.12	FL1	FV2	FL1 X_A	FL1 X_B	FV2 Y_A	FV2 Y_B	FV1 Y_A	FV1 Y_B	FL2 X_A	FL2 X_B
M2F1	This work	42.54	82.02	0.590	0.400	0.010	0.880	0.590	0.400	0.010	0.850
	Evolutionary	43.48	81.68	0.500	0.490	0.020	0.800	0.660	0.350	0.010	0.790
M2F2	This work	43.53	79.66	0.590	0.400	0.010	0.880	0.590	0.400	0.010	0.850
	Evolutionary	34.79	73.03	0.601	0.390	0.020	0.899	0.630	0.330	0.010	0.890

From the Table 3 we observe, again, a very good estimation of the flow of the interconnection streams, that is possible to generate just considering the easy separation index and the feed composition is used. Also, it is clear that estimation of the compositions of the interconnections streams is an excellent estimation. Basically, the interconnection flows FL1 and FV1 are pseudo binaries (light and intermediate), while FV2 and FL2 have the intermediate component in major proportion. This observation applies to mixture with an easy separation index major than the 1.

If the mixture has an easy separation index of 1, then the tendency found in the interconnection flows FL1 and FV1 stands; however, the interconnection flows FV2 and FL2 are also pseudo binaries mixtures integrated by the intermediate and heavy components.

5. Conclusions

A short and optimal design procedure for dividing wall distillation columns has been presented. The procedure considers as key variables the interconnection flows: flows and compositions. In order to get information about these variables, we generated Pareto fronts of seven mixtures of different natures, four feeds and three recoveries. The analysis of these variables shows that we can make a very simple relation for the flows of the interconnection flows as a function of the easy separation index and the feed composition. We found that for this correlation the recoveries do not have influence. Also, the analysis of all this information, allows us to generate estimations of the compositions of each interconnection stream, as a function of the easy separation index. This information is used in order to design a dividing wall column, or even a Petlyuk configuration.

The information generated from the analysis of the Pareto front was applied to two ternary mixtures, not considered to generate the Pareto fronts. Results show that we can get very good estimations of the flows and compositions of the interconnection flows, with very simple equations and values.

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