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Kaibel Column: Modeling and Optimization

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Abstract

In this work, we propose a rigorous model for the simulation and optimization of a dividing-wall configuration known as Kaibel column (KC). The rigorous model, based on the well-known MESH equations of a conventional Continuous Distillation Column (CDC), is separated into four sets of equations that represent the main sections of the column: above, below, left side, and right side sections of the dividing wall, including secondary sections formed by the trays in between the side feed and outlets. The non-linear programming optimization of this rigorous model is performed in order to determine the Kaibel Column potential benefits, such as energy savings and greater purities for the middle products within a single column. The proposed steady-state Kaibel Column performs the separation of a quaternary methanol, ethanol, propanol, and butanol mixture while minimizing a total annual cost function using the reflux ratio, vapor and liquid rates, the product rates, and the heat duties as the manipulated variables of the system. The results show that the Kaibel Column is able to reduce the energy consumption in the reboiler and condenser by more than 40 % compared to the conventional sidedraw continuous counterpart. Also, the reduction in the number of trays of the dividing wall proves to be an important factor since small reductions in energy consumption were observed. The model was coded in Pyomo and solved using the NLP solver IPOPT.

Keywords: Dividing Wall Columns, Kaibel Columns, NLP Optimization.

1. Introduction

Over the last decades, the study of new dividing wall configurations has been addressed with the purpose of solving the inherent problem of the traditional distillation processes: their high energy consumption. One of the innovative solutions to overcome this energy problem is the use of intensive configurations, such as Dividing Wall Distillation Columns (DWDC), created by the addition of a wall that splits the column in two sections. While its construction and control might still represent a challenge, this configuration has proven to generate savings up to 30 % in energy consumption and, in some cases, savings in the capital and investment costs by reducing the number of distillation columns needed to perform a multicomponent separation (Dejanovic et al., 2010). Among these divided columns different configurations have been proposed where the Kaibel Column (KC) (Kaibel, 1987) is considered a promising option since it can replace a sequence of two, three or more distillation columns needed to purify a multicomponent mixture (Yildrim et al., 2011) since it is able to separate more than three products within a single column (Kiss et al., 2012). The simulation and optimization of this multi-product configuration has been performed first by using commercial software to simulate the column then by the use of an external algorithm which performs the optimization. These results have shown for KC good controllability properties and energy savings (Qian et al., 2016, Tututi-Avila et al., 2017) but no rigorous open-source model has been reported for its study.

In this paper, we propose a model to simulate and optimize a Kaibel Column to obtain the system variable profiles that minimize a total annual cost while producing four high purity products: methanol, ethanol, n-propanol, and butanol. The proposed equations are presented in Section 3 while the case study and operational conditions are given in Section 2. Finally, the results are presented in Section 4 followed by the Conclusions in Section 5.

2. NLP Problem Statement

In a general form, the problem is stated as follows. Given a Kaibel Column configuration and a desired final product purity, a feed mixture of NC components is to be separated into NC high-purity products while minimizing the total annual cost function. To accomplish this goal the reflux ratio, the vapor flowrate, the liquid distributors, and the heat duties are used as the manipulated variables in the NLP optimization problem, allowing the purification (to some pre-specified tolerance) of the NC components in the feed.

3. Model Equations

The proposed model for the KC was obtained by modifying the mass and energy balances on the internal trays of a conventional Continuous Distillation Column (CDC) with two side outlets, S_1 and S_2. This model is given in Eq.(1) to Eq.(13) with the objective function (TAC) in Eq.(14) which comprises the cost of the column shell, the internal sieve trays, and heat exchangers costs. The proposed set of MESH equations is split into four main sections: above and below the dividing wall and the left and right sections of the dividing wall (section 1 and 2, respectively). Some secondary sections, such as the trays in between the side feed F and the side outlets S_1 and S_2, are also considered in the model. All these sections can be seen in the KC scheme in Figure 1. Due to space limitations, only the mass balances per component are given here and will have to be further modified by the reader to complete the MESH equations of the model. The model mass balances equations are given in the next order: reboiler and vapor distributor in Eq.(1) and Eq.(2), starting tray of the dividing wall in section 1, side feed tray, and ending tray of the dividing wall in section 1 in Eq.(3) to Eq.(5), starting tray of the dividing wall in section 2, side outlet 1, side outlet 2, and ending tray of the dividing wall in section 2 in Eq.(6) to Eq.(9), and liquid distributor

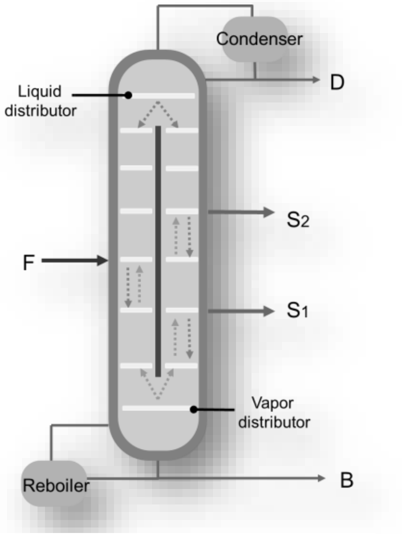

Figure 1. Kaibel Column.

and condenser in Eq.(10) and Eq.(11). The total mass balances are obtained when the liquid and vapor compositions terms are removed from Eq.(1) to Eq.(13) while the energy balances are obtained when the liquid and vapor composition terms are replaced by the liquid and vapor enthalpy terms in Eq.(1) to (13). The vapor compositions, composition summation, vapor-liquid equilibrium constants, activity coefficients (UNIQUAC), and vapor and liquid enthalpy equations are also included and solved in the model. The Total Annual Cost (TAC) is given in Eq.(14). The trays are numbered from the bottom to the top of the column, with tray *1* the reboiler and tray *NT* the condenser.

$$0 = \left(L_{j+1} + F - S_1 - S_2\right)x_{j+1,i}^1 - V_j y_{j,i} - B x_{j,i} \tag{1}$$

$$\begin{aligned} 0 = \left(L_{j+1}^1 + F\right)x_{j+1,i}^1 + \left(L_{j+1}^2 - S_1 - S_2\right)x_{j+1,i}^2 + V_{j-1}y_{j-1,i} \\ - \left(L_j + F - S_1 - S_2\right)x_{j,i} - V_j^1 y_{j,i} - V_j^2 y_{j,i} \end{aligned} \tag{2}$$

$$0 = \left(L_{j+1}^1 + F\right)x_{j+1,i}^1 + V_{j-1}^1 y_{j-1,i} - \left(L_j^1 + F\right)x_{j,i}^1 - V_j^1 y_{j,i}^1 \tag{3}$$

$$\begin{aligned} 0 = \left(L_{j+1}^1 + F\right)x_{j+1,i}^1 + \left(L_{j+1}^2 - S_1 - S_2\right)x_{j+1,i}^2 + V_{j-1}y_{j-1,i} \\ - \left(L_j + F - S_1 - S_2\right)x_{j,i} - V_j^1 y_{j,i} - V_j^2 y_{j,i} \end{aligned} \tag{4}$$

$$0 = \left(L_{j+1}^1 + F\right)x_{j+1,i}^1 + V_{j-1,i}^1 y_{j-1,i} - \left(L_j^1 + F\right)x_{j,i}^1 - V_j^1 y_{j,i}^1 \tag{5}$$

$$0 = L_{j+1}^1 x_{j+1,i}^1 + V_{j-1}^1 y_{j-1,i}^1 - \left(L_j^1 + F\right)x_{j,i}^1 - V_j^1 y_{j,i}^1 + F x_{F,i} \tag{6}$$

$$0 = L_{j+1}^1 x_{j+1,i} + V_{j-1}^1 y_{j-1}^1 - L_j^1 x_{j,i}^1 - V_j^1 y_{j,i}^1 \tag{7}$$

$$0 = (L_{j+1}^2 - S_1 - S_2)x_{j+1,i}^2 + V_{j-1}^2 y_{j-1,i} - (L_j^2 - S_1 - S_2)x_{j,i}^2 - V_j^2 y_{j,i}^2 \tag{8}$$

$$0 = (L_{j+1}^2 - S_2)x_{j+1,i}^2 + V_{j-1}^2 y_{j-1,i}^2 - (L_j^2 - S_1 - S_2)x_{j,i}^2 - V_j^2 y_{j,i}^2 - S_1 x_{j,i}^2 \tag{9}$$

$$0 = L_{j+1}^2 x_{j+1,i}^2 + V_{j-1}^2 y_{j-1,i}^2 - \left(L_j^2 - S_2\right)x_{j,i}^2 - V_j^2 y_{j,i}^2 - S_2 x_{j,i}^2 \tag{10}$$

$$0 = L_{j+1}^2 x_{j+1,i} + V_{j-1}^2 y_{j-1,i}^2 - L_j^2 x_{j,i}^2 - V_j^2 y_{j,i}^2 \tag{11}$$

$$0 = L_{j+1} x_{j+1,i} + V_{j-1}^1 y_{j-1,i} + V_{j-1}^2 y_{j-1,i}^2 - L_j^1 x_{j,i} - L_j^2 x_{j,i} - V_j y_{j,i} \tag{12}$$

$$0 = V_{j-1} y_{j-1,i} - L_j x_{j,i} - D x_{j,i} \tag{13}$$

$$TAC = C_H Q_{Reb} + C_c Q_{Con} + \frac{I_R (I_R + 1)^{PL}}{(I_R + 1)^{PL}} (C_{shell} + C_{int} + C_{HE}) \tag{14}$$

The notation is: *j* are the trays, *i* are the components, superscripts 1 and 2 represent the section 1 (left side) and 2 (right side) of the dividing wall, *x* and *y* are the liquid and vapor composition, S_1 and S_2 are the side outlets flowrate, *D* and *B* are the distillate and bottoms flowrate in kgmol/h, *F* is the side feed flowrate in kgmol/h, *L* and *V* are the liquid and vapor flowrate in kgmol/h, Q_{Reb} and Q_{Con} are the energy consumption in the reboiler and condenser in kW, *rr* is the internal reflux ratio, I_R and *PL* are the interest rate and plant life, C_H, C_C, and C_{HE} are the costs of heat and cold utilities and the heat exchangers while C_{shell} and C_{int} are the costs of the column shell and internal with installation.

3.1. Case Study

The study of the KC is performed by separating an equimolar quaternary mixture of methanol (1), ethanol (2), n-propanol (3), and butanol (4). The separation is carried out with the objective of obtaining four high-purity products with the following specifications: product flowrates higher than 0.2 kgmol/h and final compositions higher than 0.99 for the four components. The proposed model was solved under steady-state conditions with the operational conditions given in Table 1 and considering the following degrees of freedom: the condenser and reboiler duties, the product flowrates, the reflux ratio, the liquid and vapor rates, and the liquid distributor. The vapor distributor is assumed to be constant since it is known to be a very difficult variable to control during the column operation (Yildrim et al., 2011). The problem is initialized by performing the simulation of the KC column (*obj=1*) while using the warm start option in IPOPT. This simulation is followed by the solution of the NLP optimization problem using the TAC as the objective function. In order to compare the energy consumption in the reboiler and condenser, the KC results are compared to the results obtained from the optimization of a conventional CDC under the same operational conditions. The proposed KC and the CDC NLP models were written in Pyomo and solved using IPOPT.

4. Results

The optimization results for the KC and the conventional CDC for the quaternary methanol-ethanol-propanol-butanol mixture separation are presented in Table 2. The four high-purity products specification of 0.99 was achieved by the KC while the CDC was able to achieve it only in the distillate and bottom products with middle products that only reached a purity of 0.93. The KC comprises a system of 8,226 equations solved in 481 seconds while the CDC comprises a system of 5,258 equations solved in 190 seconds. Even though the middle products were not highly purified by the CDC, the conventional column energy consumption is higher than the heat duty consumed by the KC column. This is consistent with the behavior observed for other mixtures, where savings around 14 % are observed with respect to the conventional CDC separation sequence (Tututi-Avila et al., 2017). For this separation case, a comparison between the results in Table 2 shows that KC reduces the energy consumption in the reboiler by 42.14 %,

Table 1. Operating conditions for the KC.

Number of trays	70
Side outlets trays, S_1-S_2	20-40
Side feed tray, *F*	35
Dividing wall starting tray, *dws*	10
Dividing wall ending tray, *dwe*	50
Vapor distributor, dv_1	0.60
Initial vapor flowrate, *V*	5
Initial liquid composition	$x^{0}_{i\,i}$
(1) Methanol	0.25
(2) Ethanol	0.25
(3) n-Propanol	0.25
(4) Butanol	0.25
Side feed liquid composition	$x^{0}_{i\,i}$

followed by a reduction of 45.6 % in the condenser. The change in the position of the dividing wall slightly affects the energy consumption when the number of dividing-wall trays is reduced (34 dividing-wall trays, from tray 13 to tray 47 of the main column), slightly higher energy savings of 42.6 % in the reboiler and 46 % for the condenser are observed when compared to the base case (40 dividing-wall trays, from tray 10 to 50 of the main column). On the other hand, the addition of trays on the dividing-wall will lead to a reduction on the energy efficiency by moving from energy savings from the base case of 42.14 % for the reboiler to 41.73 while the condenser changes from 45.6 % to 45.13 %. These changes might not seem significant but it is important to point out the importance on the selection of the dividing wall trays and their position. We can therefore say that the proposed KC model gives a consistent solution that can predict the behavior of the different non-linear variables involved in this intensified distillation configuration.

To study the behavior of the variables in the system we present the KC liquid composition profiles in Figure 2. In Figure 2(a) the composition profiles above and below the dividing wall with section 1 of the dividing column are given, while Figure 2(b) shows the profiles above and below the dividing wall with section 2 of the dividing column. In Figure 2(a) we observe how the propanol composition is diluted by the side feed *F* on tray 35, with smaller composition values on the trays below it. On the other hand, section 2 profiles in Figure 2(b) show how the four products achieve the desired purity by keeping a reflux ratio value close to 1 and a temperature profile on the internal trays of the column close to the pure component boiling points, allowing for a better separation compared to section 1. Notice the remixing effect on the middle products after their removal from tray 20 and 40, observed in the shaded area in Figure 2(b). This dilution could lead to small thermal inefficiencies in the KC, reducing the energy savings. But it is important to point out that for this particular case, the remixing effect is not significant since we are already achieving energy savings when compared to the solved CDC. However, in order to reduce these inefficiencies in further examples we would have to perform a more in depth study on the optimal position of the side outlets.

Table 2. Results for the CDC and the KC.

	CDC	KC		
Dividing Wall Trays		10-50*	13-47	9-51
Q_{Reb}	61.628	35.652	35.405	35.911
Q_{Con}	56.950	30.997	30.764	31.249
Reflux ratio	0.963	0.937	0.937	0.937
Side feed	0.855	0.802	0.801	0.803
Distillate/Bottoms	0.203[1]/0.199[1]	0.200/0.202	0.200/0.201	0.200/0.202
Side outlet 1	0.227[2]	0.200	0.200	0.200
Side outlet 2	0.224[2]	0.199	0.200	0.199
Liquid distributor, dl_1	-	0.50	0.50	0.50

* Base case. [1] Methanol and butanol composition in *D* and *B* is 0.99.

[2] Ethanol and propanol composition in S_1 and S_2 is 0.93.

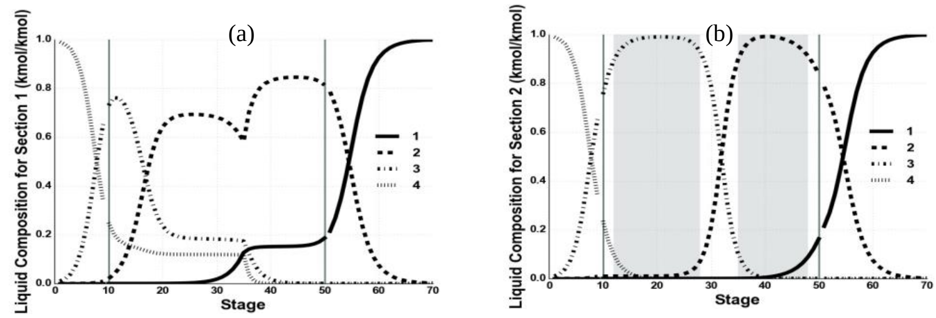

Figure 2. Liquid composition profiles of the Kaibel Column. (a) Liquid composition profiles of the main column with section 1 of the dividing wall. (b) Liquid composition profiles of the main column with section 2 of the dividing wall.

5. Conclusions

In this work, we proposed a model for the simultaneous simulation and optimization of a Kaibel Column for the separation of high-purity products of a methanol-ethanol-propanol-butanol mixture. In order to study the behavior of all the variables involved in a distillation process and the energy efficiency of a KC, a simulation was performed first, followed by the NLP optimization problem that minimize the total annual cost function under fixed flowrate and composition product specifications. To be able to compare and define possible energy savings, a conventional Continuous Distillation Column was also solved. By comparing these two columns we observe that the KC proposed model shows accurate profiles by achieving energy savings of around 42 % in the reboiler and 45 % in the condenser for the base case, while the reduction of 2 trays in the dividing wall increased this savings by an extra 0.50 %, proving how important it is to decide the number of trays and their position in a distillation configuration. These results show that the proposed model can be used as an accurate option for the solution of Kaibel Column configurations.

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