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# A Shortcut Design for Kaibel Columns Based on Minimum Energy Diagrams

Maryam Ghadrdan,<sup>a</sup> Ivar J. Halvorsen,<sup>b</sup> Sigurd Skogestad<sup>a</sup>

<sup>a</sup>Norwegian University of Science and Technology, Chemical Engineering Department, 7491, Trondheim, Norway; e-mail: ghadrdan@nt.ntnu.no, skoge@nt.ntnu.no <sup>b</sup>SINTEF ICT, Applied Cybernetics, N-7465 Trondheim, Norway; e-mail: ivar.j.halvorsen@sintef.no

# Abstract

In this paper, a shortcut procedure is proposed to design a 4-product dividing-wall column. It is based on the information derived from  $V_{min}$  diagram. This has the advantage of having more meaningful guesses for energy requirements and impurity flows in the column. An example is used for illustration.

Keywords: Shortcut design, Kaibel Column, Minimum Energy Diagrams

# 1. Introduction

The dividing wall column is a single-shell column, divided into two parts with a prefractionator and a main section with a sidestream product, which is capable of separating mixtures into three high-purity products. Compared to conventional schemes with two columns in sequence, it needs less energy, capital and space. In this paper we study the Kaibel column, which has been modified to have two sidestream products and can separate the feed into four high-purity prodicts using a single shell.

In terms of design, there are 12 degrees of freedom for the Kaibel column. These are the number of theoretical stages in each of the 6 sections plus the 6 operational DOFs. This is for a given feed rate (e.g. F=1 mol/s) and the column diameter will depend on the chosen feed rate.

Some shortcut methods have been proposed for design of 3-product columns (Triantafyllou and Smith 1992; Sotudeh and Hashemi Shahraki 2007). One approach is to extend the existing methods of conventional columns to dividing wall columns by representing the Petrlyuk column by three conventional columns. Another approach is to use more direct insight into the properties of the Petlyuk column and make use of the  $V_{min}$  diagram. We use this approach.The method consists of the following steps: First the  $V_{min}$  diagram is sketched. The advantages of using  $V_{min}$  diagram in design are discussed in detail in section 3. In section 4, the minimum flowrates in all parts of the column will be calculated. Assuming that actual vapour flow is somewhat higher (around 10%) than the minimum value, the actual flows will be calculated.  $N_{min}$  will be calculated based on Underwood equation, except for the section between two side streams for which the Fenske equation is used.

## 2. V<sub>min</sub> diagrams

Figure 1 shows the V<sub>min</sub> diagram for the Methanol/Ethanol/1-Propanol/1-Butanol system  $(c_1..c_4)$  which is the example considered in this paper. The peaks  $P_{AB}$ ,  $P_{BC}$  and

 $P_{CD}$  represent minimum energy for sharp product splits of the original mixture in the extended petlyuk configuration. Each peak is related to each of the common Underwood roots  $(\theta_A, \theta_B, \theta_C)$ . For a Petlyuk arrangement, the prefractionator performs the "easy" split between components A and D  $(P_{AD})$ . However, in a Kaibel-arrangement the prefractionator performs the more difficult split between components B and C. For the Kaibel column we must compute the new peaks  $P'_{AB}$  and  $P'_{CD}$  (the detailed procedure on how to get the peaks  $P'_{AB}$ ,  $P'_{CD}$  is found in (Halvorsen and Skogestad 2006)). The minimum energy in the Kaibel arrangement is given by the highest of the new peaks (here  $P'_{AB}$ ). It is obvious from this diagram that the Kaibel arrangement always consumes more energy than the full Petlyuk arrangement since  $P'_{AB} > P_{AB}$ ,  $P'_{CD} > P_{CD}$  and trivially:  $P'_{AB} > P_{BC}$  and  $P'_{CD} > P_{BC}$ .



Figure 1. (a)  $V_{min}$  diagrams for equimolar feed of the first 4 simple alcohols,  $\alpha = [6.616 \ 4.343 \ 2.256 \ 1]$ , (b) Schematic of the column

In case of inequal peaks in petlyuk configuration, there will be an optimality region which is a line from preferred split point to the point where the two peaks become equal (Halvorsen 2001). The optimality region will be like a square below B/C peak (as shown in Figure 1), which is impurity allowance in prefractionator. We assume that the recovery of  $c_1$  in the top of prefractionator and the recovery of  $c_4$  in the bottom of prefractionator are 1 and 0 respectively  $(r_{c_1,T} = 1, r_{c_2,T} = \beta_1, r_{c_3,T} = \beta_2, r_{c_4,T} = 0)$ . The net flow rates which enter the main column for the top and bottom will be calculated from  $\sum z_i F \beta_i$  and  $\sum z_i F (1 - \beta_i)$  respectively. The common underwood roots in the prefractionator are calculated from equation (1). The solution obeys  $\alpha_1 \geq \theta_1 \geq \alpha_2 \geq \theta_2 \geq \cdots \geq \alpha_N$ 

$$1 - q = \sum \left( \alpha_i z_i / \alpha_i - \theta \right) \tag{1}$$

$$V_{\min,p} = \sum_{i} (\alpha_i z_i F / \alpha_i - \theta) \times \beta_i$$
<sup>(2)</sup>

 $\langle \mathbf{n} \rangle$ 

The vapour flow rate which corresponds to  $\theta_2$  will be the minimum requirement for prefractionator because it characterizes the B/C split.

## 3. Select product purites

Selection of product purities is based on the economical analysis and customer needs. Note that the minimum vapour flow for the Kaibel column is the same as the maximum of the minimum energy required for any pair of product splits, and the highest peak shows the most difficult split. It is clear that we can think of extra energy in one section and then talk about either increasing the product recovery or designing with lower number of trays. It is shown that overfractionating one of the products makes it possible to bypass some of the feed and mixing it into the product while retaining the constraints on the products (Alstad, Halvorsen et al. 2004). In addition, the impurities in products can be guessed from  $V_{min}$  diagram. For example, the highest peak in the  $V_{min}$  diagram determines the component that may appear as impurity in the side stream during optimal operation. So, care should be taken in specifying the product impurities. Figure 2 shows the trends of changes in side stream impurity ratios as functions of splits and impurities coming from the prefractionator for the example studied in this paper. This proves the fact about the impurity flows which go to the sidestream and also helps to put some feasible values in mass balance equations.

By writing the total and component mass balances for the whole column to get the minimum allowable flows inside each section we will have 8 equations (component balances) and 20 unknowns, which means that 12 variables should be set in order to solve the mass balance equations.

$$Fz_{c_i} = Dx_{c_i,D} + S_1 x_{c_i,S_1} + S_2 x_{c_i,S_2} + Bx_{c_i,B}$$
 and  $\sum x_{i,Str_j} = 1$ 

where  $x_{m,N}$  means mole fraction of component *m* in Product *N*.

We assume that the composition of the component in two sections away from which it is the main product, is nearly zero, e.g. the compositions of the lightest component in side stream 2 and bottom stream. By doing so and also specifying the composition of the main product in each product stream, there remains two DOF to be specified. It is shown that specifying two composition specifications in a product stream may lead to problems (Wolff and Skogestad 1995). This means that the impurity can not be chosen as an arbitrary value. Figure 3 shows the contours of the ratios of impurities in side streams around the optimum as functions of vapour and liquid split. It can be read from the figures that for example the specifying two ratios as any arbitrary specification may be infeasible. So, one important issue is the allowable variables which can be set for product impurities so that the mass balance equations lead to feasible solution.

#### 4. Minimum allowable and actual internal flows

The other internal flow rates for the prefractionator section and main column will be calculated easily from balances around different junctions. The common roots in the prefractionator section, will be the active roots in the main section. The minimum vapour flow rate value for each section in the main column can be calculated from equation (2), by simply substituting the proper feed flow, feed composition and recovery values for each section (for example  $z_{i,2} = (F/D_1) \times \beta_i z_{i,F}$ ,  $q_2 = -L_{\min,p}/D_1$ ,  $\beta_i (\sec 2) = Dz_D/D_1 z_{D_i}$  for top section of the main column).

Now, we can continue with assuming the actual vapour flow needed for the whole column to some extent (we assume 10%) higher than the minimum value and then calculate the actual internal flows.

0.





Figure 3. Contours of the impurity ratios in side streams as functions of liquid and vapour split

The liquid and vapour splits are defined as the ratio of the strams going to the prefractionator to the amount coming to the joint.  $r_L = L_1/L_2$  and  $r_V = \overline{V_1}/\overline{V_3}$ .

The other internal flows on two sides of the wall will be calculated based on the splits. Since the internal flows should be greater than the minimum flows, there are some constraints which should be met. Otherwise, the equations will not have proper roots related to relative volatilities.

$$r_{L} < (L_{2} - \bar{L}_{\min,2})/L_{2} \qquad r_{L} > \max\left(L_{\min,1}/L_{2}, (\bar{L}_{\min,1} - qF)/L_{2}\right)$$
(3)  
$$r_{V} > \max\left(\overline{V}_{1,\min}/\overline{V}_{3}, (V_{1,\min} - (1 - q)F)/\overline{V}_{3}\right) \qquad r_{V} < (\overline{V}_{3} - V_{3,\min})/\overline{V}_{3}$$

Section four is the section between two side-streams and it's considered to have total reflux and the number of trays will be calculated directly from Fenske equation. Since Fenske equation is based on assuming equal compositions of liquid and vapour streams at top and bottom of prefractionator, -which is not the case for DWC-, we derive the minimum number of trays from Underwood equation. A few iterations are done to reach a desired value for number of trays and energy requirement. The equation below is used for calculating the number of trays in each section.  $x_{i,L}$  is the composition of the entering stream to prefractionator, which is calculated from pinch point equations (Halvorsen 2001).

$$N = \log \left( \left( \frac{\sum \frac{\alpha_i x_{i,D}}{\alpha_i - \phi_2}}{\sum \frac{\alpha_i x_{i,D}}{\alpha_i - \phi_1}} \right) / \left( \frac{\sum \frac{\alpha_i x_{i,L}}{\alpha_i - \phi_2}}{\sum \frac{\alpha_i x_{i,L}}{\alpha_i - \phi_1}} \right) \right) / \log \left( \frac{\phi_2}{\phi_1} \right)$$
(4)

## 5. Conclusion

Designing the complex columns is not as straightforward as the conventional columns. In this paper we have presented a method for shortcut design of Kaibel column based on Vmin diagram. By plotting the contours of the objective value as a function of the two operational DOFs, we can get more information about the behaviour of the column close to the optimum and do the optimal design based on the rigorous model.

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