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Design and simulation of divided wall column: Experimental validation and sensitivity analysis

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ABSTRACT

This article deals with design and simulation of divided wall column. Design parameters are provided to the rigorous simulation in the ProSimPlus® software. The results show that the procedure can determine parameters quickly in the case studies and can give a good initialization for rigorous simulation. Secondly, a pilot plant has been design, built and operated in our laboratory. The pilot plant will provide necessary experimental evidence to validate the previous procedure. Ternary mixture and four-component mixture of alcohols have been used in our pilot plant in steady state conditions. The results show that the composition of products, composition and temperature profile along the column are in very good agreement with simulation results. Finally, in order to determine the optimal parameters of divided wall columns, the effects of the structural parameters of the divided wall column such as the height of the wall, the vertical position of the wall and number of stages of each section are analyzed. Ternary diagram is used as an indicator both in showing what the most economical configuration is and in showing the distillation boundary.

1. Introduction

The divided wall column (DWC) has many known advantages, and many design methodologies for DWC's have been published over the last years. Almost all papers that have been published were restricted to ternary mixtures with three products, sharp separations, saturated liquid feed, constant flowrate and constant relative volatility. The design of divided wall columns or fully thermally coupled distillations is more complex than traditional distillation because it has more degrees of freedom. A number of papers have been published on the subject which focus on the calculation of the minimum vapor requirement and determined the number of stages in the various column sections. Triantafyllou and Smith [4] published a design oriented shortcut method for three products in a divided wall column based on the Fenske–Underwood–Gilliland–Kirkbridge model (FUGK). In this paper, they presented a method to decompose a divided wall column into a three-traditional-column model. By using the decomposition method, they assume that heat transfer across the column wall can be neglected, hence making the divided wall column equivalent to a fully thermally coupled distillation. The prefractionator is considered like a traditional column if a partial condenser and a partial reboiler are used. The main column can be represented as two traditional columns if we assume a total reboiler for the upper part of the main column and a total condenser for the lower part of the main column. The interconnecting streams are considered as the feed flowrates with superheated vapor and sub-cooled liquid conditions, respectively. The FUGK method can be applied to determine operational and structural parameters for each column. The minimum number of equilibrium stages can be determined by the Fenske equation, the minimum reflux ratio can be determined by using the Underwood equation, the number of stages can be determined by the Gilliland method when choosing operating reflux ratio, and feed location can be determined by the Kirkbride method. The reflux ratio of the prefractionator is adjusted until its number of stages equals the number of the side section. The recoveries in the prefractionator column are optimized for the minimum vapor flowrate or the minimum number of stages.

Amminudin et al. [1,2] proposed a semi-rigorous design method based on equilibrium stage composition concept. Certain assumptions are as follows: constant molar overflow, constant relative volatility, and estimation of component distribution at minimum reflux. Their design procedure starts from defining the products composition, and works backward to determine the design parameters required to achieve them. Therefore, firstly, by using

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Nomenclature

A, B, C	Ternary mixture (A is the most volatile component and C is the least volatile component)
D	Top product flowrate (kmol h^{-1})
F	Feed flowrate (kmol h^{-1})
L	Liquid flowrate in the rectifying section (kmol h^{-1})
$\overline{L}$	Liquid flowrate in the stripping section (kmol h^{-1})
N	Number of stages
q	Quality of the stream
R	Reflux ratio
R_L	Liquid split between prefractionator and main column
R_V	Vapor split between prefractionator and main column
S	Side product flowrate (kmol h^{-1})
V	Vapor flowrate in the rectifying section (kmol h^{-1})
$\overline{V}$	Vapor flow rate in the stripping section (kmol h^{-1})
x	Mole fraction at the product stream
W	Bottom product flowrate (kmol h^{-1})
z	Mole fraction at the feed stream

Subscripts

1	Column I
2	Column II
3	Column III
b, c, d, e	sections separated by dividing wall
HK	Heaviest key component
LK	Lightest key component
min	minimum value
R	Rectifying section
S	Stripping section

Greek symbols

α	Relative volatility of component
τ	Recovery ratio of the component
$\theta, \theta', \theta''$	Roots of Underwood's equation
ω_G	Gas velocity (m s^{-1})
ρ_G	Gas density (kg m^{-3})

the method of Van Dongen and Doherty [18], a feasible product distribution is estimated for the composition of the top, middle and bottom products, the minimum reflux ratio and the minimum boil-up ratio. Any distillation operation lies between the two limits of total reflux and minimum reflux ratios. At total reflux ratio, the number of stages is minimized and energy consumption is maximized. At the minimum reflux ratio, the number of stages is maximized and energy consumption is minimized. Therefore, a product distribution must be chosen between the two conditions. Secondly, using the equilibrium stage concept the number of stages, flow rates, feed stage and side stream location for the fully thermally coupled distillation are estimated.

An approximate design procedure for fully thermally coupled distillation column is proposed by Kim [11]. The Fenske equation is applied to the main column to determine minimum number of stages. However, the author believed that the design of the prefractionator cannot follow the Fenske equation because the end compositions are unknown. Therefore, a stage-to-stage computation is proposed. Then, the number of stages in the system is taken as twice the minimum number of stages. The minimum vapor flowrate was determined by the Underwood equation. The liquid flowrate of the main column is determined by checking the compositions of the products. Clearly, they take twice the minimum number of stages as the number of theoretical trays is considered to be equal to two times the minimum number of stages. It is not always true.

Halvorsen and Skogestad [7,10] proposed the V_{min} diagram method to determine the minimum energy consumption. To use the method, they assume constant molar flowrates, constant relative volatilities, and an infinite number of stages. Firstly, the V_{min} diagram is drawn based on the Underwood equation. The minimum energy requirement for separation of a feed mixture of n components into n pure products is given by:

$$V_{min}^{Petlyuk} = \max \sum_{i=1}^{j} \frac{\alpha_i z_i F}{\alpha_i - \theta_j}; j \in \{1, n-1\}$$

Here: θ_j are the $n-1$ common Underwood roots found from:

$$1 - q = \sum_{i=1}^{n} \frac{\alpha_i z_i}{\alpha_i - \theta}$$

Underwood roots obey $\alpha_1 > \theta_1 > \alpha_2 > \theta_2 > \ldots > \theta_{n-1} > \alpha_n$

where: q is liquid fraction in the feed (F) and z is the feed composition

Secondly, they choose the actual flowrate around 10% and the minimum number of stages was calculated based on the Underwood equation.

Calzon-McConville et al. [5] presented an energy efficient design procedure for optimization of the thermally coupled distillation sequences with initial designs based on the design of conventional distillation sequences. In the first step, it is assumed that each column performs with specified recoveries of components of 98% (light and heavy key components) and by using the shortcut method (FUG model), the number of stages of conventional distillation schemes are obtained. In the second step, the stage arrangements in the integrated configurations are obtained; finally, an optimization procedure is used to minimize energy consumption. The energy-efficient design procedure for thermally coupled distillation sequences is applied not only for the separation of ternary and quaternary mixtures but also for the separation of five or more component mixtures.

Sotudeh and Shahraki [14,15] proposed a shortcut method for the design of a divided wall column based only on the Underwood equation because authors believe that using the Fenske equation for calculating the minimum number of stages is not adequate for designing divided wall columns. The theoretical number of stages can be calculated by using the basic Underwood equation. In this method, the number of stages in the prefractionator is set to be the same as in the side section. Clearly, we cannot know that the number of stages of prefractionator is correct or not. Moreover, the paper does not carry out simulations to confirm the method.

Ramirez-Corona et al. [13] presented an optimization procedure for the Petlyuk distillation system. The procedure used the FUG model to determine the structural design of the divided wall column as well as the mass and energy balances, the thermodynamic relationships, and cost equations. The objective function was set as the minimization of the total annual cost. In the procedure, they estimated the composition of the interconnection streams between the prefractionator and the main column by solving the feed line and the operating line equations.

$$y_i = \left(\frac{q}{q-1}\right) x_i - \frac{x_{i,D}}{q-1}$$

$$y_i = \left(\frac{R}{R+1}\right) x_i + \frac{x_{i,D}}{R+1}$$