

Influence of dividing wall position on performance of dividing wall column with vapor feed

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Abstract. In this paper, a rigorous method is developed for optimal design of dividing wall column (DWC) considering tray hydraulics and used to investigate the influence the vapor fraction in the feed on the horizontal positioning of the dividing wall and on the performance of the column. The pseudo-transient model by Ma et al. and an equation-oriented approach to distillation column optimization considering stage hydraulics by Li et al. are employed in the rigorous optimization. With the method, a DWC for separating a ternary mixture of n-pentane, n-hexane and n-heptane is employed to illustrate the influence of the vapor fractions in the feed on the partition positioning in the DWC, where off-center diagonal partition wall (swaged-wall design) is allowed, in terms of its economic performance. The results show that the vapor fraction in the feed has strong effect on the optimal positioning of the partition.

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Introduction

Dividing wall column (DWC) for ternary distillation has outstanding advantages in terms of energy saving and investment cost reduction comparing with traditional two-column sequences ^[1]. However, due to the coupling nature of the distillation configuration, more freedoms or decision variables must be considered for optimal design of a DWC ^[2]. As new decision variables for the DWC, liquid split ratio and vapor split ratio for distributing the liquid and vapor phases respectively to the two sides of the dividing wall, have been shown critical effect on the performance and, ultimately, the cost of the separation. In the optimal design of DWC, the liquid split ratio can be adjusted as an operating variable, but the vapor split ratio is spontaneously adjusted by the pressure drop on both sides of the partition ^[3, 4], and the adjustment depends on the partition position and hydraulic conditions on both sides of the partition wall^[5-7]. The feed thermal condition, that is, the vapor fractions in the feed has strong effect on the vapor and liquid flow rate and, consequently, on the hydraulic conditions in the column sections of DWC. Therefore, considering the change of the feed vapor fraction is of great importance in the optimal design of DWC. However, such an investigation has not been reported yet to our knowledge.

The difficulty of rigorous and systematic optimal design of DWC can be attributed to the increased complexity of the optimization problem by the inclusion of the hydraulic models, and the convergence issue of Newton type method in the solution of the problem. Moreover, simultaneously optimization of stage numbers of the multi column sections in the DWC must be addressed and results in a complex mixed-integer nonlinear programming (MINLP) problem. Aiming at solving the problem, Ma et al. ^[8] developed a new pseudo-transient (PT) distillation model by transforming the initial value problem of the Newton-type solution into the initial condition problem in the solution of the differential-algebraic equations (DAE) system and employing the bypass efficiency model of Dowling and Biegler for stage number optimization^[9,10]. The easy-to-solve DAE effectively improves the robustness of the convergence of the Newton method. Li Feng et al. ^[5] successfully applied this method to optimization of distillation columns, in clouding the DWC, considering tray hydraulics.

In this paper, based on the rigorous simulation and optimization method of distillation column considering tray hydraulics proposed by Li Feng et al. ^[5], the DWC with different vapor fraction feeds is optimized. The influence of the vapor fraction in the feed on the structural parameters including the position of the partition is investigated, and the advantages of different positions of the partition and the reasons for this advantage are quantitatively analyzed through rigorous simulation calculation.

Model and optimization algorithm

Basic PT Rigorous Equilibrium Distillation Model

To avoid conversion issue in a Newton type method, the optimization of DWC in the present work is enabled by employing the pseudo-transient model and solution procedures proposed by Ma et al. ^[11]. The equilibrium stage model, or the MESH [material balance (M), phase equilibrium (E), summation (S) and heat balance (H)] equations are given in form of differential-algebra equation (DAE) system, where the material balance and energy balance equations are expressed in the form of differential equations.

Material balance equation (M):

For the normal stages:

$$\frac{dM_i^j}{dt} = V^{j+1}y_i^{j+1} + L^{j-1}x_i^{j-1} - V^jy_i^j - L^jx_i^j \quad (1)$$

For the feed stage:

$$\frac{dM_i^j}{dt} = V^{j+1}y_i^{j+1} + L^{j-1}x_i^{j-1} - V^jy_i^j - L^jx_i^j + (F_1 + F_v)z_i \quad (2)$$

where F_v and F_1 are the vapor flow rate and liquid flow rate, respectively, in the feed.

For the intermediate product side-draw stage:

$$\frac{dM_i^j}{dt} = V^{j+1}y_i^{j+1} + L^{j-1}x_i^{j-1} - V^jy_i^j - L^j(1 + S_f^j)x_i^j \quad (3)$$

where S_f refers to the ratio the product with-draw over the liquid flow.

Phase equilibrium equation (E):

$$y_i^j = k_i^j x_i^j \quad (4)$$

Summation equation (S):

$$\sum_{i=1}^{i=c} x_i^j = 1; \quad \sum_{i=1}^{i=c} y_i^j = 1 \quad (5)$$

Heat balance equation (H):

For the normal stages:

$$\frac{dH^j}{dt} = V^{j+1}h_v^{j+1} + L^{j-1}h_L^{j-1} - V^jh_v^j - L^jh_L^j \quad (6)$$

For the feed stage:

$$\frac{dH^j}{dt} = V^{j+1}h_v^{j+1} + L^{j-1}h_L^{j-1} - V^jh_v^j - L^jh_L^j + F_1h_1 + F_vh_v \quad (7)$$

For the intermediate product with-draw stage:

$$\frac{dH^j}{dt} = V^{j+1}h_v^{j+1} + L^{j-1}h_L^{j-1} - V^jh_v^j - L^j(1 + S_f^j)h_L^j \quad (8)$$

For the feed, a parameter γ_f can be defined as the fraction of vapor flow in the feed:

$$\gamma_f = F_v / (F_v + F_1) \quad (9)$$

To determine the final solution of the differential-algebraic equations, Ma et al. proposed a simple linear pseudo hold-up correlation ^[11]:

$$L^j = C_L M_L^j; \quad V^j = C_V M_V^j \quad (10)$$

where C_v and C_L are constants and assigned the value 1800 h⁻¹ as recommended by Ma et al ^[11].

Tray Hydraulics Model

Tray hydraulics model depend on the type of tray. In this paper sieve tray is adopted and the hydraulics formula proposed by Bennett et al. ^[12] is used to calculate the stage pressure drop. The pressure drop of a single tray is composed by the following three parts:

Liquid inventory on a tray:

$$h_L = \phi \left[h_w + C \left(\frac{Q_L}{\phi} \right)^{2/3} \right] \quad (11)$$

Passage of vapor through dry tray perforations:

$$h_d = \frac{0.499}{c_v^2} \frac{\rho_v V_H^2}{\rho_L g} \quad (12)$$

Formation of vapor bubbles:

$$h_\sigma = \frac{4\sigma}{g\rho_L d} \quad (13)$$

Partition Position Parameter

The basic structure of DWC is shown schematically in figure 1(a), where six column sections are involved, and the part composed by sections II and IV is termed as the pre-fractionator, the other sections compose a main column. Non-circular trays appear in DWCs because of the presence of partition, but due to the lack of hydraulic model of non-circular trays, in this paper we adopt the method of Dejanović et al. [7] to equate non-circular trays to circle trays. The variable describing the horizontal position of the partition is represented by the ratio of the cross-sectional area of the pre-fractionation column to the whole column cross sectional area:

$$\beta = \frac{S_l}{S_l + S_r} = \frac{\theta - \sin \theta}{2\pi} \quad (14)$$

where S_l and S_r are the column cross sectional areas of the left and right sides of the partition, respectively; θ is the angle subtended by the partition wall. Given the definition, when $\beta=0.5$, the partition is in the middle position, otherwise it is biased toward the pre-fractionation column ($0 < \beta < 0.5$) or the main distillation column ($0.5 < \beta < 1$).

Optimization Algorithm

In order to investigate the effect of different partition positions, two different DWCs are designed, one with the same upper and lower partition positions, called off-center straight dividing wall column (straight-wall design), and the other with different upper and lower partition positions, called diagonal off-center dividing wall column (swaged-wall design). The schematic diagram is shown as in Figure 1^[4,13]. In the two DWCs, column sections II and IV in the figure are the distillation section and stripping section of the pre-fractionator column respectively; section I is the common distillation section and VI is the common stripping section.

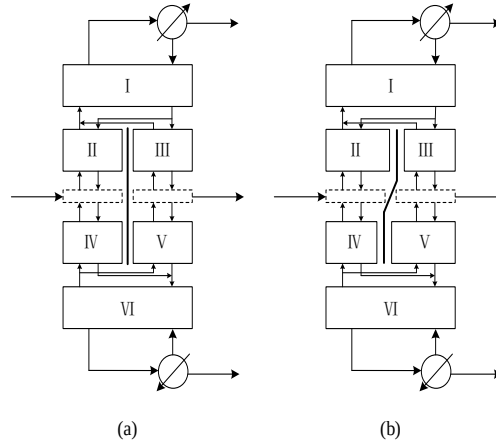


Fig. 1 Schematic diagram of the DWC model a. Straight wall b. Swaged wall.

In this study, the total annual cost (TAC) is used as the criterion to optimize the decision variables to obtain the optimal structure that satisfies the minimum TAC, while satisfying the hydraulics constraints. The decision variables to be optimized include the number of trays of the six sections (N_i), reflux ratio (RR), boilup ratio (BR), side-draw fraction (S_i), vapor split ratio (R_v), liquid split ratio (R_L), operating pressure (P), column diameter (D) and partition position parameters (β). The optimization process of DWC is shown in Figure 2.

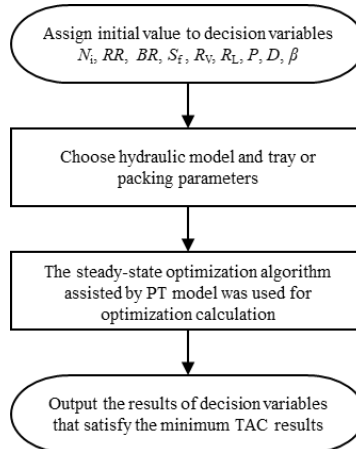


Fig. 2 Design framework of a DWC.

The optimization of the stage number in this study uses the bypass efficiency model proposed by Dowling et al. [11, 12]. Bypass efficiency parameter (ε_j) is used to describe the existence or non-existence of tray j , that is, if ε_j approaches 1 or 0, it indicates the existence or non-existence of the tray respectively. The sum of all bypass efficiency parameters is the total number of stages. Finally, the steady-state optimization algorithm assisted by pseudo-transient models is used to complete the simultaneous optimization of all variables, and the steady-state optimization is accomplished using the Hypsqp solver in Aspen Custom Modeler.

Case study

In this study, separation of the mixture of *n*-pentane (A), *n*-hexane (B) and *n*-heptane (C) is employed to illustrate the influence of partition positions on feed in vapor in DWC. The feed conditions and product requirements are shown in Table 1. SRK method is used as the thermodynamic model. The models in section 1.2 are used to calculate the pressure drop of the trays. Taking the minimum TAC as the criterion for the optimization, the structural and operating parameters are optimized simultaneously. The investigations are made for two feed conditions. In Case 1 the feed is the saturated liquid (feed vapor fraction is 0), and in Case 2 the feed is the saturated vapor (feed vapor fraction is 1).

Table 1.
Feed condition and product request.

Parameter	Value
feed flow rate/kmol·h ⁻¹	300
feed composition	A:B:C=1:1:1
feed vapor fraction	0/1
feed pressure/kPa	101.325
product request	A:0.987,B:0.98,C:0.987

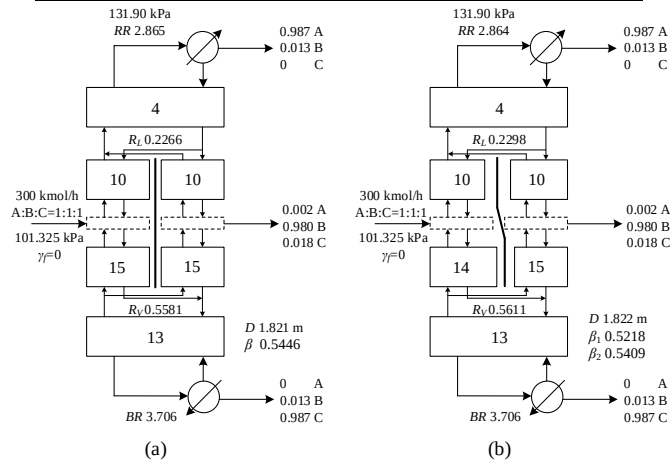
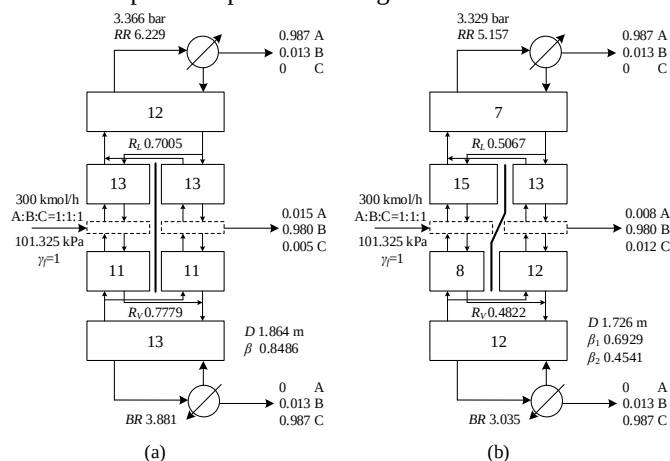


Fig. 3 Rigorous simulation results of DWC with feed in liquid (Case 1).

For Case 1, the rigorous optimizations for both the straight-wall design(Case 1.a) and swaged-wall design(Case 1.b) are carried out, the results are shown in figure 3, and the related costs are listed in Table 2. The results show that the partition position parameter β for the straight-wall design is 0.5446(figure 3.a), and the upper and lower partition position parameters β_1 and β_2 for the swaged-wall design are respectively 0.5218 and 0.5409 (figure 3.b), and β_1 and β_2 are very close, and β_2 is roughly the same as β of the straight-wall design. β_2 is higher than β_1 because larger space for more liquid is provided in the section IV. The other structural parameters and operating parameters of the two structures are almost the same, and from Table 2, Case 1.a and Case 1.b have the similar cost and TAC results. It shows that for liquid feed, whether the partition position is diagonal off-center has little effect.

**Fig. 4** Rigorous simulation results of DWC with feed in vapor (Case 2).

The two configurations are also optimized with vapor feed(Case 2), and the corresponding calculation results are listed in Figure 4, and the related costs are listed in Table 2, where Case 2.a is for the straight-wall design and Case 2.b is for swaged-wall design. The results show that the structural parameters and operating parameters are significantly different from each other. β for straight-wall design is 0.8492 (figure 4.a), and β_1 and β_2 for swaged-wall design are 0.6931 and 0.4496 (figure 4.b). It can be found in Figure 4 that the vapor and liquid split ratios are significantly different. R_V and R_L of straight-wall design are 0.7779 and 0.7005, respectively, and R_V and R_L of swaged-wall design are 0.4822 and 0.5067, respectively.

Table 2.
Comparison of the costs of the DWC

Cost/10 ⁴ \$	Case1.a	Case1.b	Case2.a	Case2.b
Capital Cost	93.53	93.56	114.38	98.15
Column cost	52.17	52.21	60.84	52.96
Condenser Cost	25.12	25.20	16.38	14.92
Reboiler Cost	16.17	16.16	37.16	30.27
Operating Cost	75.44	75.47	74.90	58.76
Condenser Energy Cost	3.14	3.14	5.33	4.57
Reboiler Energy Cost	72.30	72.32	69.57	54.18
TAC	106.61	106.66	113.02	91.48

For Case 2.a, the vapor flow rate increases significantly in section II of pre-fractionator column and the partition position is required to move towards right to leave larger cross sectional area for section II. Because of the configuration of the straight-wall design (section II and section IV have the same column diameter), the cross sectional area in section IV is increased with section II. A consequence is that the section IV is more prone to weep because of the unnecessary enlargement of the cross sectional area. As a result, a bigger vapor split ratio is required so that more vapor from the bottom of column enters the section IV. As for the swaged-wall design, i.e. Case 2.b, the upper and lower partition position parameters can be adjusted independently so that the vapor split ratio can be optimized more freely. This explains why the swaged-wall design has a lower operating cost in both the condenser and the reboiler, as shown in Table 2. When the feed vapor fraction is 1, the TAC of swaged-wall design is 19.06%

lower compared with the straight-wall design, and the capital and operating costs are saved by 14.19% and 21.55%, respectively. The total vapor and liquid load in swaged-wall design are lower than the straight-wall design. As the column diameter is determined by the maximum vapor flow, the column diameter of the swaged-wall design is smaller than the straight-wall design. As seen from Figure 4, the vapor and liquid split ratio of the swaged-wall design is smaller than that of the straight-wall design, that is, both the vapor and liquid loads of the pre-fractionation column are reduced, and both of the main column are increased, making the number of trays in the main column of the swaged-wall design reduced. This leads to a reduction in capital cost. As the total vapor and liquid loads are reduced, the reflux ratio and boilup ratio are reduced, and so the operating cost is reduced.

Conclusions

As analyzed in the paper, the rigorous optimization method considering tray hydraulics can be effectively applied to the optimal design of the DWC column with vapor feed. It is shown that the optimal design on the partition position plays an important role on affecting the performance of a DWC when the feed is vapor phase. It is also shown that the diagonal off-center dividing-wall configuration is necessary when off-center dividing-wall is considered. Therefore, when the feed is turned from liquid phase to vapor phase, a DWC should be re-designed considering the swaged-wall configuration to achieve a lower cost.

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