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Rate-based design of integrated distillation sequences

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Abstract

In this work, the separation of a ternary mixture by different distillation sequences is analyzed with respect to feasible energy and cost savings for various feed compositions. For this purpose, a method combining short-cut and rate-based models is used, which allows fast determination of relevant set-ups and operating parameters, with due account of kinetic limitations. For a ternary alcohol system, five different distillation sequences are studied regarding energy demand, total capital and operating costs. It is shown that thermally coupled columns and dividing all columns provide significant energy and cost savings as compared to conventional distillation sequences.

Keywords:

distillation, short-cut modeling, rate-based modeling, energy consumption, cost calculation, thermally coupled columns, process integration

1. Introduction

Process intensification represents one of the most promising trends in chemical engineering and process technology. It results in reduction of equipment and plant size, improvement of process efficiency and safety, decrease of waste and energy consumption and, consequently, a better process economics.
Distillation remains a widely used and the most energy intensive step in chemical and process industries [1]. Therefore, distillation-related consumption has a significant impact on overall plant profitability. In the last decades, various strategies have been adopted to improve the efficiency of distillation systems. These efforts are particularly important considering permanent energy cost increase.

2. Distillation of ternary mixtures

When multicomponent mixtures should be separated by means of distillation, serial sequences of distillation columns can be applied. For ternary mixtures with components A, B and C, these sequences are realized either as a direct or as an indirect configuration (Fig. 1).

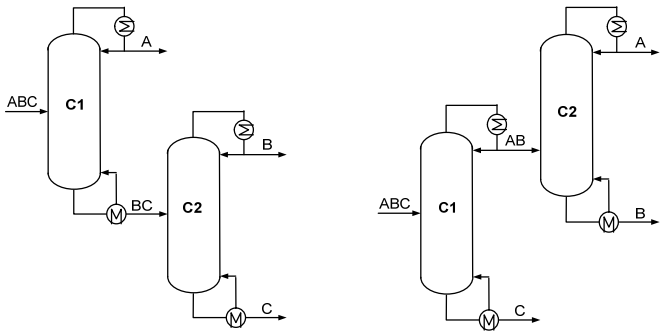

Figure 1. Conventional column arrangements for separation of ternary mixtures: direct sequence (left); indirect sequence (right)

In conventional distillation sequences, the components are separated in correspondence with their boiling temperatures, which often requires high energy input. From the standpoint of thermodynamics (and, accordingly, efficient energy use), an optimal distillation arrangement for the separation of a ternary mixture requires three columns (Fig. 2, left) [2]. In the first column, the lightest (A) and the heaviest (C) components are separated very efficiently, due to their high relative volatilities. The intermediate boiling component (B) appears in both top and bottom streams of column C1 and is separated in the second and third columns (C2 and C3).

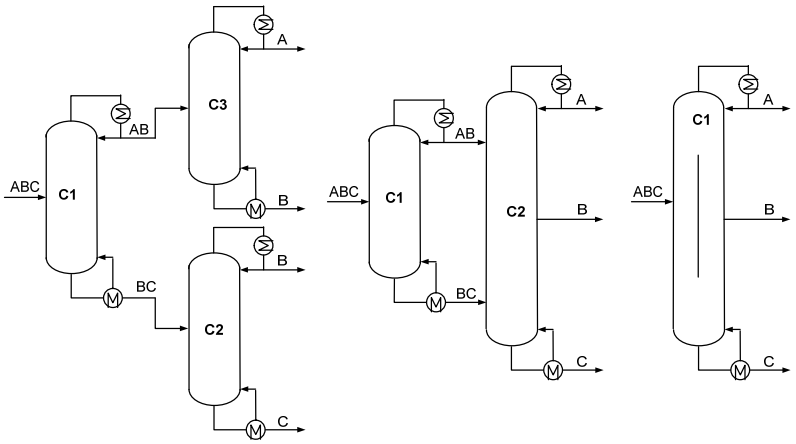

Figure 2. Simple column arrangement for separation of ternary mixtures: direct/indirect sequence (left); prefractionator configuration (centre); dividing wall column (right)

Although the direct/indirect sequence shown in Fig. 2 (left) is thermodynamically more attractive than the direct or indirect arrangements, its set-up requires an additional column, a reboiler and a condenser. This increases the total energy demand (as the mixture has to be evaporated and condensed in each single column). The reboiler of the column C3 and the condenser of column C2 can be avoided by thermally coupling of both columns; thereby a reduction of equipment units can be achieved (Fig. 2, centre). This sequence is called prefractionator configuration. The highest degree of integration is realized by the dividing wall column (Fig. 2, right), when a vertical partition (wall) is introduced into a distillation column. This unit enables the separation of a ternary mixture within one single column shell.

3. Modeling and Simulation

For the present study, five different distillation sequences are considered, namely, the direct configuration, the indirect configurations, the direct/indirect combined sequence, the prefractionator configuration as well as the dividing wall column. The feed used for the simulation is a ternary mixture methanol-isopropanol-butanol, whereas different feed compositions are investigated (Table 1). The boiling points of the pure components at atmospheric pressure are 64°C (methanol), 82°C (isopropanol) and 117°C (butanol).
The feed flow rate is 10 m^3/hr, the feed temperature is 78.5°C and column pressure is atmospheric. Purities around 95 mol% for all products are required.
As the first step, short-cut models available in the process simulation tool ASPEN Plus™ [3] are used to perform preliminary design of separation sequences including column set-up (number of stages, feed location) and operating conditions (reflux ratio, distillate-to-feed ratio). These short-cut

methods (Underwood, Fenske and Gilliland, see [4]) are very simple, therefore, a reasonable testing of their results by a more accurate approach is desirable.

Table 1. Investigated feed compositions in mol%

feed mixture	1	2	3	4	5
butanol	20	30	33	45	10
isopropanol	50	50	33	10	80
methanol	30	20	34	45	10

For this reason, the second step is the application of the rate-based approach which enables a direct account of the process kinetics [5]. By this method, actual rates of multicomponent mass and heat transport between liquid and vapor phase can be considered. The rate-based models are implemented in the simulation environment ASPEN Custom Modeler^{TM} [6,7]. These models are further extended by the capital and operational cost calculation according to [8,9]. The optimal diameter of each column is determined with the software tool SULPAK^{TM} 3.3 [10] as a function of flow rates within the column and mixture properties (e.g., liquid and vapor density). For the description of the thermodynamic properties, the UNIQUAC model is applied.

4. Simulation results by the rate-based approach

For the rate-based simulations, basic design parameters obtained by the short-cut methods are used. The total number of theoretical stages obtained from the short-cut models has to be converted into a packing height using the HETP-value (height equivalent to theoretical plate). For the selected packing Sulzer BX^{TM}, a HETP-value of 0.25 m is chosen. For the reflux ratio, the value 1.2 times the minimum reflux ratio is taken, because, close to this point, the total costs (incl. operating and capital costs) are reported to be nearly minimized [11]. The rate-based simulations confirm that the product purities are reached in the column configurations given by the short-cut models. In addition, information about the column profiles, e.g., temperature and concentration, as well as heat duties and costs, is obtained.
The simulation results for the composition of feed mixture 1 (cf. Table 1) are presented in Fig. 3 and 4. Fig. 3 demonstrates that the prefractionator configuration and the dividing wall column require almost 40% less energy than the conventional configurations.

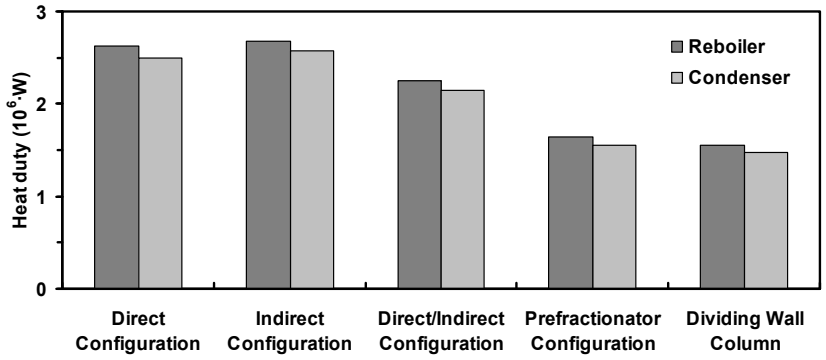

Figure 3. Reboiler and condenser heat duties for different distillation sequences

Figure 4 shows the annualized capital (linear amortization over 10 years) and operating costs for each distillation sequence. The costs are related to the maximum value for all sequences, which is the total capital cost of the indirect configuration. It can be seen that the capital cost of the dividing wall column is 40% lower than that of the cheapest conventional configuration (direct configuration). Savings can also be realized with the prefractionator configuration, with costs reduction about 32%. The annualized capital costs are low compared to the operating costs (< 15%), which demonstrates that significant cost savings can only be realized by more energy efficient processes.

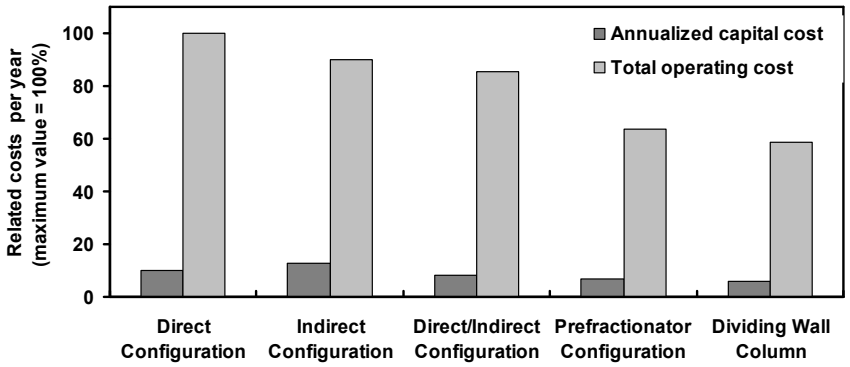

Figure 4. Related capital and operating costs for different distillation sequences

It is worthy of note that the conventional direct and indirect configurations permit a certain heat integration which improve their efficiency [12]. This integration has not been considered in our work yet.

5. Conclusions and future work

The present study deals with different distillation sequences including those based on thermal coupling and integration principles, with the aim to reduce energy consumption and total costs. A combination of short-cut and rate-based models is applied for a rapid determination of the required set-up and operating conditions and obtaining detailed information about the process behavior and costs. The ternary alcohol mixture methanol-isoporpanol-butanol is chosen as a test system. For this ideal system, the product purities predicted by the short-cut models are confirmed by the rate-based simulations. In addition, the investigations show that the capital and operation costs can be significantly lowered using the prefractionator configuration as compared to conventional column arrangements. The application of the high-integrated dividing wall column leads to a further decrease of the costs. The conventional direct and indirect configurations are generally less efficient.
Future work will be focused on industrial and non-ideal systems. This requires more intricate short-cut models, which are able to treat non-idealities. Besides, feasible heat integration between single columns should be considered.

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