Optimal Operation of Vapor-recompressed Middle Vessel Batch Distillation

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Abstract

This article focuses on the optimal operation of an energy-integrated batch distillation configuration. The vapour-recompressed middle vessel batch distillation (VR-MVBD) employs a heat pump system wherein the latent heat available with the top vapour is utilized to vaporize the reboiler liquid. The optimal operation policy is formulated through the maximization of an operational performance index which combines separation and energy efficiency. Specifically, a dynamic optimization problem is solved by exploiting the various degrees of freedom, such as the initial feed distribution and trajectories of vapor and reflux flows. A reduced model governing the dynamics of the VR-MVBD column is employed for better computational efficiency. Lastly, the effectiveness of the proposed approach is demonstrated using a simulation case study of cyclo-hexane, n-heptane, and toluene separation. It is shown that the proposed optimal operation policy doubles the performance index of the system as compared to the base case.

**Keywords**: Batch distillation, energy-integration, heat pump, dynamic optimization

* 1. Introduction

Batch distillation, due to operational flexibility and low capital investment, is one of the most preferred separation processes in the chemical industry. However, it also encounters several challenges like long batch time and low energy efficiency. In recent years, effective utilization of energy in batch distillation has been the focus of research activity. To this end, numerous energy-integrated batch distillation configurations have been proposed, such as vapor-recompressed batch distillation (VRBD) (Johri et al., 2011), heat-integrated batch distillation (Nakaiwa et al., 2003), middle vessel batch distillation (MVBD) (Hasebe et al., 1992) and batch divided wall columns (Jana, 2016). Subsequently, Babu et al. (2012) integrated the MVBD and VRBD schemes to propose a vapor-recompressed middle vessel batch distillation (VR-MVBD) configuration to further improve energy efficiency of batch distillation. In VR-MVBD, the overhead vapor is thermally coupled with the reboiler using a heat pump. In order to generate a favorable thermal driving force, a compressor is employed to raise the condensation temperature of the top vapor above the bubble point of the bottom liquid.

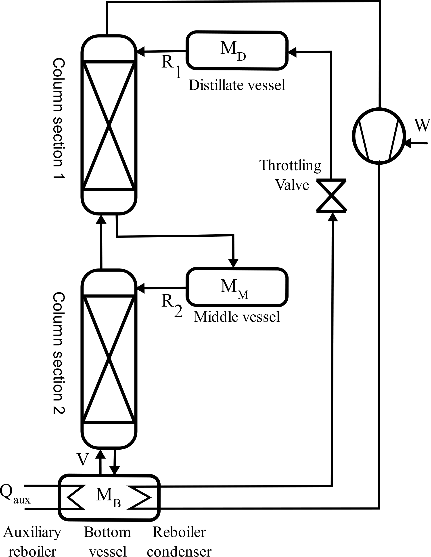
In the context of VRBD, Parhi et al. (2019) developed an optimal reflux policy using a multi-objective optimization framework and demonstrated substantial reduction in energy consumption and CO2 emission. Similarly, Vibhute and Jogwar (2020) obtained an optimal operation policy for a VRBD column using dynamic optimization and closed-loop control. Along similar lines, for a MVBD configuration (without vapor recompression), it has been shown that significant performance improvement can be achieved through dynamic optimization by balancing separation and energy efficiency (Beniwal and Jogwar, 2023). In the case of VR-MVBD, additional interactions due to vapor recompression add a new dimension to this trade-off as the savings due to energy integration are also dependent on the top and bottom composition profiles and thus the extent of separation. However, the existing study on VR-MVBD by Babu et al. (2012) considers constant reboiler duty and vessel holdup throughout the batch and results in suboptimal performance (as demonstrated in this paper). Motivated by this, the present work focuses on the optimal operation of a VR-MVBD configuration by manipulating input variables, such as initial feed distribution and trajectories of vapor and reflux flows. To quantify performance of the column, an economic performance index is defined to capture separation and energy efficiency. Thereafter, a dynamic optimization problem is solved to maximize this performance index by utilizing the available degrees of freedom. The rest of the paper is organized as follows. Section 2 describes the considered system and presents the governing dynamic equations. The next section focuses on the formulation of the dynamic optimization problem. In section 4, a case study involving the separation of a mixture consisting of cyclo-hexane, n-heptane, and toluene is presented to illustrate the effectiveness of the proposed approach.

Figure 1: Vapor-recompressed middle vessel batch distillation (VR-MVBD) configuration

* 1. VR-MVBD configuration

As shown in Figure 1, this configuration consists of two column sections and three vessels for the separation of a ternary mixture. The vapor leaving the top of column section 1 is compressed using a compressor to increase its dew point temperature. The latent heat of this compressed vapor is utilized in the reboiler (bottom vessel) to generate vapor required for separation. The rest of the heat requirements are met via an auxiliary reboiler. The condensate leaving the reboiler-condenser is throttled and sent to the distillate vessel. Fresh feed can be introduced through any/all of the vessels. The VR-MVBD column is operated under total reflux, and the three products, based on their relative volatility, accumulate in the distillate, middle, and bottom vessel. The batch ends when the products in all three vessels reach their desired purity specification. For simplicity, let us consider constant holdup on each tray and constant relative volatility throughout the column. Accordingly, Eq. (1) captures the dynamics of this system.

|  |  |
| --- | --- |
|  | (1) |

where , , and represent molar holdup, liquid phase mol fraction, and vapor phase mol fraction, respectively. , , and represent the vapor flow rate and reflux flow rates from the distillate and middle vessel, respectively. Subscripts , , and refer to the distillate vessel, middle vessel, and bottom vessel, respectively. Subscripts , , and denote tray, stage number (from the top of the column), and component j, respectively. Subscripts and refer to the last stage of column section 1 and 2, respectively. The vapor and liquid phase mole fractions are related to each other through the vapor-liquid equilibrium relationship and stage efficiency definition. Specifically, at *i*th stage,

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| --- | --- |
|  | (2) |

where represents the relative volatility, the subscript represents the equilibrium value, and represents Murphree tray efficiency.

During the operation, the overhead vapor and the bottom vessel liquid get enriched in the more volatile and less volatile components, respectively. Therefore, to maintain a constant thermal driving force between the bubble point temperature of the reboiler liquid () and the dew point temperature of the compressed vapor (), the compressor is operated at variable speed. The required compression ratio () and the corresponding compressor power () are estimated using the following equations.

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| --- | --- |
|  | (3) |

where , , and represent the temperature of the overhead vapor, specific heat ratio, and isentropic efficiency of the compressor, respectively. and represent outlet and inlet pressure, respectively. Subsequently, the auxiliary reboiler duty is computed using the following equation.

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| --- | --- |
|  | (4) |

where and represent latent heat and specific heat capacity, respectively.

* 1. Optimal operation

Optimization of an energy-integrated distillation configuration attempts to achieve desired separation with minimum energy consumption. Thus, to generate an optimal operating policy, it is essential to include both production and energy consumption for performance quantification. Accordingly, an overall performance index (OPI) is defined as the ratio of the value of the separated products to the cost of energy consumed during separation. The OPI can be computed using the following expression:

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| --- | --- |
|  | (5) |

where and represent *i*th vessel holdup and batch processing time, respectively. , , and represent the value of the product collected in the *i*th vessel, cost of the auxiliary reboiler duty and cost of the compressor duty, respectively.

The optimal operation problem involves obtaining the trajectory of input variables to maximize a performance index while incorporating practical constraints. Therefore, a dynamic problem is formulated to obtain the optimal operating policy for the VR-MVBD configuration. Maximization of OPI is considered as an objective function. The decision variables () are the trajectory of vapor flow rate (), and reflux flow rates from distillate and middle vessel ( and ). A piecewise constant input policy is considered. As the tray holdup is very small as compared to a vessel holdup, the dynamic system given by Eq. (1) is stiff. Singular perturbations are used to derive non-stiff realization of these dynamic equations and the corresponding DAE system is used during dynamic optimization (Beniwal and Jogwar, 2023). This reduces the number of dynamic variables as well as allows for using a larger time step for discretization. The corresponding dynamic optimization problem is given as follows.

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| --- | --- |
| Subject to: Reduced dynamic model for VR-MVBD  Input bounds:  Input move constraints:  Vessel holdup constraints:  Purity constraints ∀ products:  Feasible composition constraints: | (6) |

* 1. Case study

Let us now illustrate this framework with an example system of cyclo-hexane, n-heptane, and toluene separation. The base case design is considered from literature (Babu et al., 2012) and slightly modified to obtain 99% purity for all the three products. The VR-MVBD column consists of total 74 trays (, ) to process 50 kmol fresh feed () with composition () of (0.1, 0.6, 0.3). Initial feed is distributed to all the three vessels in proportion to the composition (denoted as proportional feed distribution). The volatility values are , and . At the base case, the column is operated under the constant vessel holdup with a fixed vapor flow rate of 0.58 kmol/min, and the corresponding batch time is 816 minutes. A two-stage compressor system with equal pressure ratio is employed to maintain the required compression ratio. The OPI value for the base case operation is 23.31. The relative error between the reduced and full model for product composition in distillate, middle, and bottom vessel is 1.97%, 1.10% and 2.33%, respectively.

The optimization problem given by Eq. (6) is solved using the CasADi (Andersson et al., 2019) framework in MATLAB version R2022a. Implicit Euler method, with a time step of 1 min, is used to discretize the dynamic equations. The maximum and minimum value for each optimization variable is taken as 0.5 kmol/min and 1 kmol/min, respectively. Their change at any time step is restricted to kmol/min. The vessel holdups are constrained between 1.1 kmol and 45 kmol, respectively. Lastly, cost of each product, hot utility and compressor power are taken as 15 rcu/mol, 2.3 rcu/MJ and 7.0 rcu/MJ, respectively (rcu refers to relative cost unit).

Figure 2(a) shows the variation of component holdup for each vessel. Two distinct phases for holdup redistribution can be observed. Specifically, in the first phase of the operation, both the column sections are utilized to perform a relatively difficult separation between n-heptane and toluene, leading to an increase in the concentration of cyclo-hexane and n-heptane in the distillate vessel and the concentration of toluene in the bottom vessel. Subsequently, in the second phase of operation, final product purity specifications in all the vessels are achieved by transferring the partial holdup of the distillate vessel, enriched in n-heptane, to the middle vessel. The OPI value for this policy is 49.11 and corresponds to an increase of 111% from the base case.

(a) Proportional (b) Middle vessel

(c) Bottom vessel (d) Distillate vessel

Figure 2: Dynamic profiles of component holdup for various feed distributions

Subsequently, three other initial feed distribution scenarios, bottom vessel feed (conventional batch rectifier), middle vessel feed and distillate vessel feed (inverted configuration), are considered. In the case of middle vessel feed, the variation of component holdup follows similar trend to the previous case. However, as the corresponding top and bottom compositions are different, the temperature lift required in this case is slightly higher than the previous case (see Figure 3) leading to an increase in compression power. The optimal OPI value for this case is 48.95, a small decrease of 0.3% from proportional feed distribution. When the initial feed charged to the bottom vessel, there are three distinct phases of holdup redistribution as shown in Figure 2(c). The additional phase at the start of the operation includes the distribution of material to all the vessels and temporarily storing component 3, vaporized along with components 1 and 2, in the middle vessel. In phase 2, component 3 from the middle vessel is transferred back to the bottom vessel, and the distillate vessel gets enriched in components 1 and 2. Final purity specifications are achieved in all the vessels with material redistribution during phase 3. The OPI for this policy is 48.12, a reduction of 2% from the proportional feed distribution due to the extra step of holdup transfer. Similarly, feed charged to the distillate vessel also results in three operational phases and gives an optimal OPI of 45.87.

Figure 3: Dynamic profile for required temperature lift

Lastly, in order to investigate the effect of feed composition, two other feed conditions – equimolar (zF2) and lean middle component (zF3) – are considered. The corresponding optimal OPI values for each of the feed locations are reported in Table 1. It can be seen that the proportional feed distribution results in the best performance irrespective of the feed composition. This is in contrast with the normal MVBD case wherein feed to the middle vessel resulted in the best performance (Beniwal and Jogwar, 2023). This signifies the impact of coupling between energy consumption and extent of separation due to energy integration.

Table 1: Optimal OPI values for various feed composition and location

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| --- | --- | --- | --- | --- |
| **Feed location** | **Proportional** | **Distillate** | **Middle** | **Bottom** |
| (0.1,0.6,0.3) | 49.11 | 45.87 | 48.95 | 48.12 |
| (0.33,0.33,0.33) | 46.67 | 44.23 | 45.51 | 46.06 |
| (0.40,0.25,0.35) | 51.46 | 49.81 | 49.81 | 50.06 |

* 1. Conclusions

In this paper, optimal operation policy is formulated for an energy-integrated VR-MVBD system. An economic performance index (OPI) is defined to include separation and energy efficiency. It is shown that the optimal redistribution of vessel holdup results in significant performance (OPI) improvement over the base case scenario considered in previous literature. For the case study of cyclo-hexane/n-heptane/toluene separation, irrespective of the feed composition, the proportional feed distribution results in the best performance.

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