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Optimal Operation of Middle Vessel Batch Distillation using Model Predictive Control

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ABSTRACT

Middle vessel batch distillation (MVBD) is an alternative configuration of the conventional batch distillation with improved sustainability index. This article presents a comparison of model-based control approaches for MVBD column. Specifically, two control approaches - sequential (open-loop optimization followed by closed-loop control) and simultaneous (closed-loop optimization and control) are pursued. These two approaches are compared in terms of their effectiveness, overall performance, and robustness to plant-model mismatch. The effectiveness of these control strategies is illustrated using a simulation case study of a ternary mixture separation consisting of benzene, toluene and o-xylene.

Keywords: Batch distillation, model-based control, economic model predictive control

INTRODUCTION

Batch distillation is a preferred separation process for small-scale production, multi-product and high-purity separations because of its operational flexibility and cost-effectiveness. However, it also encounters challenges like long batch time and low thermodynamic efficiency. Multi-vessel (also known as multi-effect) batch distillation is an alternative configuration of the conventional batch distillation with reduced energy consumption for multicomponent separation. Middle vessel batch distillation (MVBD), as shown in Figure 1, is a special case of multi-effect distillation with a single intermediate vessel. It allows for simultaneous separation of a ternary mixture wherein relatively pure products are collected in the three holdup vessels.

Several studies have focused on optimization and control of the MVBD configuration. Hasebe et al. (1995) used vessel holdups as manipulated variables to control composition of the products in multi-effect batch distillation [1]. Wittgens et al. (1996) proposed a temperature-based feedback control structure for multi vessel column. The temperature at a particular location in each column section is controlled using reflux flows which allows for indirect adjustment of the vessel holdup [2-3]. Further, this control strategy was examined by Furlonge et al. (1999) using dynamic optimization to determine the controller gains and set points. They demonstrated existence of a trade-off between quality of temperature control and minimum energy consumption for the separation [4]. Zhu et al. (2016) investigated composition and temperature control structures for MVBD. It was found that composition control structure was unable to control the process stably [5]. Krishna et al. (2021) showed that a cascade control structure provided more effective control than a single layer feedback control for the MVBD column [6].

The MVBD is a highly interactive system with nonlinear dynamics and requires coordinated manipulation of heat input and reflux flows to achieve desired separation. The studies mentioned above underline challenges associated with implementation of traditional linear feedback controllers. For energy integrated batch distillation, Vibhute et al. (2020) demonstrated performance improvement with model-based feedback control strategies [7]. Along similar lines, model-based control configurations can be employed to MVBD to achieve desired separation and address stability and optimality of the operation.

In this paper, two types of model-based control approaches are explored for efficient operation of a MVBD column. Firstly, in a sequential approach, optimal set-point trajectory generated with offline optimization is tracked using a model predictive control (MPC). Alternatively, in the simultaneous approach, performance optimization and control are integrated using an economic MPC.

The rest of the paper is organized as follows. A brief overview of the MVBD configuration and operating principles is presented in the next section. The following section presents design of model-based control strategies for a MVBD column. Comparison of closed-loop performance of the MVBD column with these control strategies is presented using a simulation case study of benzene, toluene and o-xylene separation.

MIDDLE VESSEL BATCH DISTILLATION

As shown in Figure 1, middle vessel batch distillation consists of two column sections separated by a vessel for the separation of a ternary mixture. It works on the principle of multi-effect operation wherein vapour from one column section is used to drive the subsequent effects, thus reducing the overall energy consumption. The entire system is operated under total reflux and at the end of the batch, the three products are accumulated in the three vessels (distillate, middle and bottom vessels).

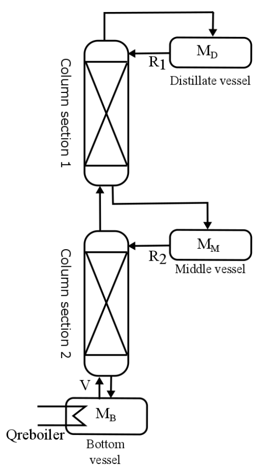


Figure 1. Middle vessel batch distillation configuration.

The mathematical model to capture the dynamics of MVBD configuration, with the assumptions of constant molar overflow and constant tray holdup, is given in Eq. (1).

Distillate vessel:

$$\frac{dM_D}{dt} = V - R_1, \qquad \frac{d(M_D x_{D,j})}{dt} = V y_{1,j} - R_1 x_{D,j}$$

Column section 1:

$$\frac{d(M_t x_{i,j})}{dt} = R_1\big(x_{(i-1),j} - x_{i,j}\big) + V\big(y_{(i+1),j} - y_{i,j}\big)$$

Middle vessel:

$$\frac{dM_M}{dt} = R_1 - R_2, \qquad \frac{d(M_M x_{M,j})}{dt} = R_1 x_{N_{T1},j} - R_2 x_{M,j}$$

Column section 2:

$$\frac{d(M_t x_{i,j})}{dt} = R_2\big(x_{(i-1),j} - x_{i,j}\big) + V\big(y_{(i+1),j} - y_{i,j}\big)$$

Bottom vessel:

$$\frac{dM_B}{dt} = R_2 - V, \qquad \frac{d(M_B x_{B,j})}{dt} = R_2 x_{N_{T2},j} - V y_{B,j} \qquad (1)$$

Here M, x, and y represent molar holdup, liquid phase mol fraction, and vapor phase mol fraction, respectively. V, R_1, and R_2 represent the vapor flow rate and reflux flow rates from the distillate and middle vessel, respectively. Subscripts D, M, and B refer to the distillate vessel, middle vessel, and bottom vessel, respectively. Subscripts t, i, and j denote tray, stage number (from the top of the column), and component j, respectively. Subscripts N_{T1} and N_{T2} refer to the last stage of column section 1 and 2, respectively.

Performance quantification

In MVBD, a ternary mixture is separated into valuable products using thermal energy. Therefore, the performance of MVBD can be effectively evaluated with the inclusion of separation and energy efficiency. Motivated by this, overall performance index (OPI) was previously defined to incorporate both production and energy consumption [9]. The OPI is defined as the ratio of the value of products obtained to the cost of energy supplied to distillation. It can be computed using the following expression:

$$OPI = \frac{\sum_{i=1}^{3}(C_i * M_i(t_{batch}))}{\int_0^{t_{batch}}[C_Q * Q_{reboiler}]dt} \qquad (2)$$

Here M_i, C_Q, and t_{batch} represent i^{th} vessel holdup, cost of the reboiler duty, and batch processing time, respectively.

MODEL BASED CONTROL STRATEGIES

In previous work, the OPI was maximized to generate optimal operation policy (initial feed distribution, vessel holdup profile, and input variable profile) for the MVBD by redistributing holdup in the three vessels [9]. Specifically, it was shown that material holdup in the column can be dynamically redistributed among the three vessels to maximize OPI for the entire batch. This optimal operation policy obtained with open-loop optimization can be directly implemented in the MVBD column. However, in the presence of external disturbances and plant-model mismatch (primarily due to simplifying modeling assumptions and vapor liquid equilibrium), a feedback control is required to maintain product purity and operational optimality.

To this end, model-based feedback control strategies can be formulated using two different approaches. In a sequential approach, offline optimization is used to derive dynamic trajectory for key process variables (vessel holdup, product purity, material and energy flows) to maximize OPI for the entire batch. Subsequently, a feedback controller is used to track this trajectory in an online manner. In the case of MVBD operation, as shown in Figure 2, this can be achieved by tracking optimal vessel holdup or product composition profiles by manipulating the reflux and vapor flows. Alternatively, in the simultaneous approach, optimization is combined with feedback control into a single step, similar to the framework of an economic model predictive control. Specifically, the typical regulatory control objective is replaced by OPI maximization and the corresponding optimal input trajectory is sent to the column in a receding horizon manner. For the MVBD operation, as shown in Figure 3, the MPC uses OPI maximization over the prediction horizon (N_p) to estimate vapor and reflux flow profile over the control horizon.

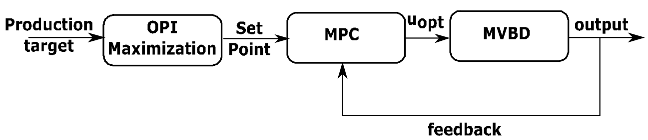


Figure 2. Sequential approach.

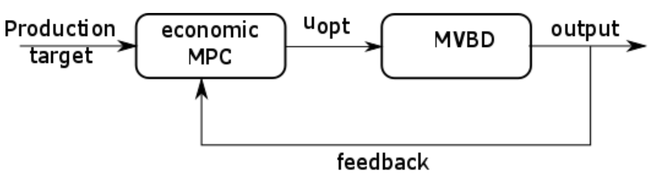


Figure 3. Simultaneous approach.

Under normal operating scenario, the sequential approach results in optimal performance. However, it meets challenges in achieving the desired product purity and/or maintain optimality in presence of significant disturbances and plant-model mismatch, since the optimal trajectory is obtained in the absence these factors. On the other hand, the simultaneous approach can effectively handle disturbances and plant-model mismatch due to active feedback. However, it can result in comparatively lower OPI since it considers a smaller prediction horizon ($N_p \ll t_{batch}$) for optimization than the sequential approach. Both these approaches are explored for MVBD column.

Let us now set up the corresponding controller formulations. At every instant, the MPC solve the following optimization problem.

$$\min_{u(t)} \; J$$

Subject to:

Dynamic model for MVBD (Eq. (1))

Input bounds: $u_{min} \leq u(t) \leq u_{max}$

Input move constraints: $\Delta u_{min} \leq \Delta u(t) \leq \Delta u_{max}$

Vessel holdup constraints: $M_{min} \leq M(t) \leq M_{max}$

Feasible composition constraints:

$$0 \leq x(t) \leq 1, \; 0 \leq y(t) \leq 1 \qquad (3)$$

The sequential and simultaneous approaches differ only in terms of their objective function.

Sequential approach

Here, optimal set-point trajectory generated with offline optimization (OPI maximization) is tracked using a model predictive control (MPC). The dynamics of the MVBD column, as shown in Eq. (1), is nonlinear; therefore a nonlinear model predictive controller (NMPC) is designed. The key variable to be tracked are composition of the products or holdup of the vessels. The corresponding objective functions are given in Eq. (4) and Eq. (5).

Vessel holdup tracking:

$$J = \sum_{i=1}^{N_p} (M_{set}(i) - M(i)) Q1 (M_{set}(i) - M(i))^T \qquad (4)$$

Product composition tacking:

$$J = \sum_{i=1}^{N_p} (x_{set}(i) - x(i)) Q2 (x_{set}(i) - x(i))^T \qquad (5)$$

Here the subscript set refers to the optimal offline trajectory, Q1 and Q2 are positive definite weighting matrices and N_P is the prediction horizon. Tracking holdup trajectory has the benefits of faster response and low sensor cost requirement but it relies on indirect control of product composition. On the other hand, tracking composition profile ensures product quality but suffers from slower response due to measurement delays and increased sensing cost (costly composition sensor or need for state estimator).

Simultaneous approach

The primary objective of the controller is to maximize OPI. However, due to the absence of any penalty term on product purity, the controller would rarely achieve the desired purity at the end of the batch. Therefore, the controller objective consists of two parts, maximization of OPI for the time window of prediction horizon and minimization of difference between desired product purity and product composition in the vessels, as shown in Eq. (6).

$$J = -w_1 * OPI(N_p) + w_2 \left(x_{D1,desired} - x_{D1}(N_p)\right) + w_3 \left(x_{M2,desired} - x_{M2}(N_p)\right) + w_4 (x_{B3,desired} - x_{B3}(N_p)) \quad (6)$$

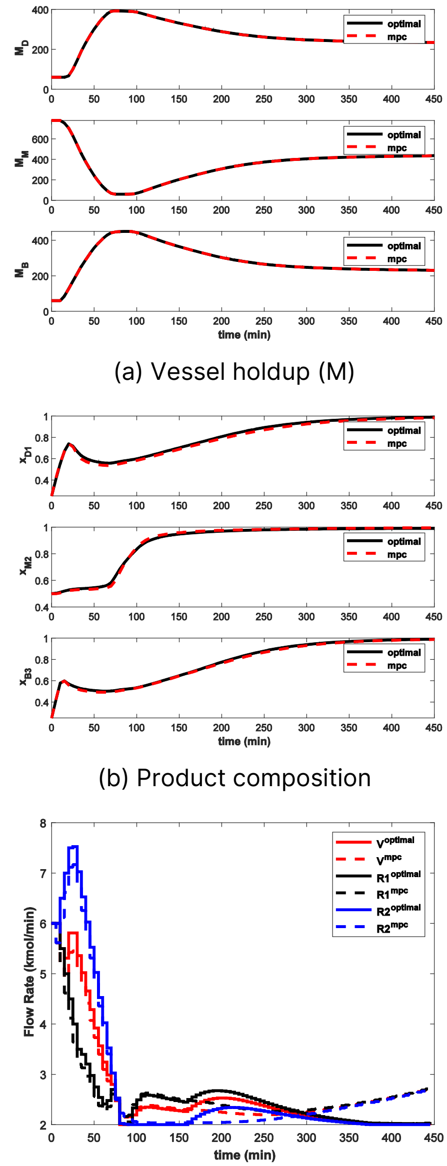
Here, the OPI is computed for the prediction horizon by replacing t_{batch} in Eq. (2) by N_p. This formulation is similar to the economic MPC as the prediction horizon for this controller is much smaller than the batch time. The tuning parameters w_1, w_2, w_3 and w_4 are adjusted to attain desired product purity with optimal performance. They also provide a trade off between quality (achieving product purity) and efficiency (optimal operation).

SIMULATION CASE STUDY

Let us now evaluate and compare the performance of these proposed control approaches with a case study of benzene, toluene, and o-xylene separation in MVBD column. The MVBD column consists of total 65 trays ($N_{T1} = 36$, $N_{T2} = 29$) to process 1000 kmol fresh feed (F) with a composition of (0.25, 0.5, 0.25). The modified Raoult's law is used to capture the vapor liquid equilibrium relationship. The activity coefficients and vapor pressure are computed using the NRTL model and Antoine equation, respectively [9]. Implicit Euler scheme with a time step of 5 min is used for the discretization of MVBD dynamics. The optimization problem is solved using the CasADi framework in MATLAB version R2022a [8]. The maximum and minimum value for each input variable is taken as 10 kmol/min and 2 kmol/min, respectively. Their rate of change across the time steps is bounded to ±0.5 kmol/min. The vessel holdups are constrained between 60 kmol and 900 kmol, respectively. Lastly, cost of each product and hot utility are taken as 15 rcu/mol and 2.3 rcu/MJ, respectively (rcu refers to relative cost unit). The OPI value of base case operation without optimization is 12.88.

In our previous work [9], we had generated optimal operation policy for the separation of above ternary mixture in MVBD column, by solving open loop optimization problem for OPI maximization. It was determined that feeding the system through the middle vessel results in optimal performance. The corresponding optimal OPI value and batch time are 26.8 and 450 minutes, respectively.

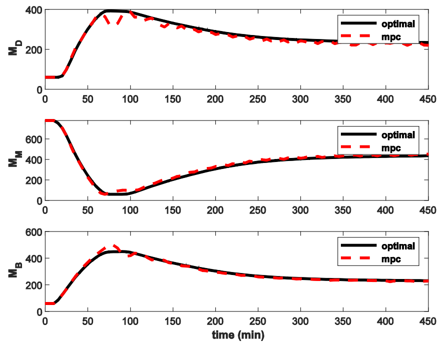
Let us first consider the sequential approach to track this optimal profile in the absence of any disturbances. Figure 4(a) shows the tracking of vessel holdup trajectory using Eq. (3) and (4). It can be observed that the nonlinear MPC is able to track the optimal trajectory of vessel holdup and desired product purity (Figure 4(b)) is achieved as well. Since the controller objective does not incorporate OPI, the optimal trajectory of vessel holdup can be achieved with various combinations of input variables. The vapour flow rate, shown in Figure 4(c), is comparatively higher than the optimal trajectory. Consequently, the OPI value with the holdup controller is 25.6, a drop of 4.5% from the openloop optimal value.



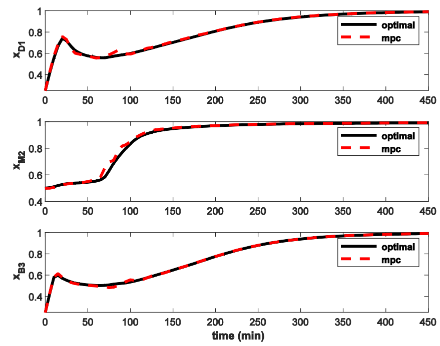
(c) Input variables

Figure 4. Dynamic response for the sequential approach with vessel holdup tracking in the absence of disturbance

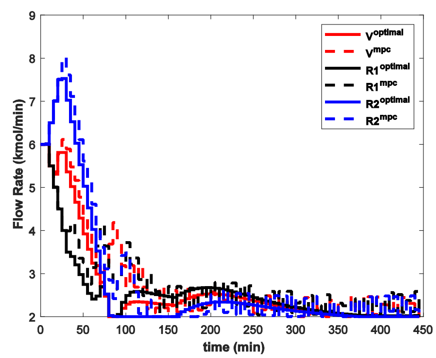
Similarly, product composition tracking using Eq. (3) and (5) is shown in Figure 5. In this case as well, the controller is able to track the optimal trajectory and reach the desired product purity. The corresponding OPI value is 24.40, a drop of 9% as compared to the openloop optimal value, due to higher vapour flow rate.



(a) Vessel holdup (M)



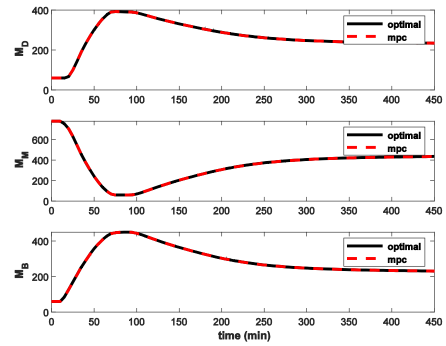
(b) Product composition



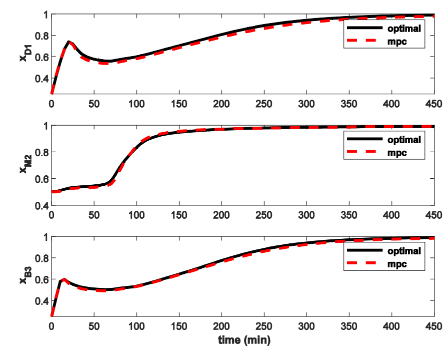
(c) Input variables

Figure 5. Dynamic response for the sequential approach with composition tracking in the absence of disturbance

Let us now consider a disturbance scenario (plant-model mismatch) in implementation of the sequential approach. It is considered that after 50 min of operation, tray efficiency for all the trays in the MVBD column is dropped by 10% due to an undetected fault. As the openloop optimization does not incorporate this disturbance, the MPC set point trajectory remains the same. In the case of vessel holdup tracking, even though the holdup tracking is done effectively, it fails to meet desired purity. The corresponding dynamic responses are as shown in Figure 6. On the other hand, in the case of product composition tracking, continuous feedback from plant ensures that at the end of the operation, desired product purity of all the components is attained. However, as the original composition trajectory is not longer optimal in this disturbance scenario, the OPI value decreases from 24.4 to 22.4, reduction of 8.2% due to presence of plant-model mismatch. The corresponding dynamic responses are depicted in Figure 7.



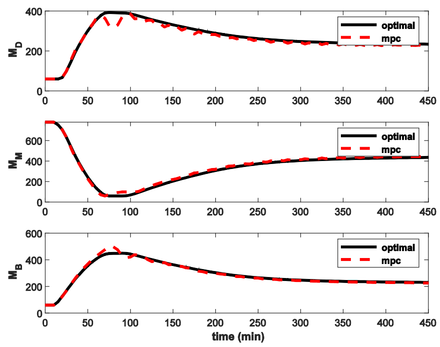
(a) Vessel holdup (M)



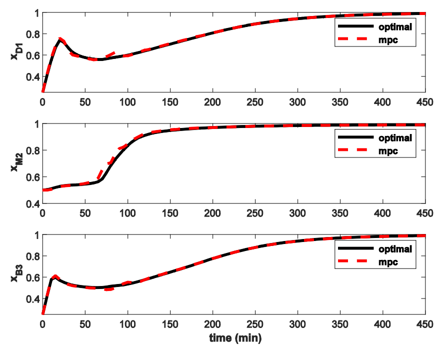
(b) Product composition

Figure 6. Dynamic response for the sequential approach with vessel holdup tracking in the presence of disturbance

Let us now assess the performance of the simultaneous approach. A nonlinear MPC is implemented using Eq. (3) and (6). Tuning parameter values are selected as $w_1 = 9 * 10^{-4}$, $w_2 = 44 * 10^{-4}$, $w_3 = 7.55$, $w_4 = 13.2$ to achieve good balance between purity attainment and performance optimization. The dynamic response of the controller in the absence of any disturbance is shown in Figure 8. Similar to the sequential approach, this controller is also able to achieve the desired product purity at the end of the batch. However, it can be observed from Figure 8(a) that the simultaneous approach is not able to capture the holdup distribution profiles obtained with open loop optimization. Previously [9], it was shown that OPI maximization requires two phases of vessel holdup redistribution for the optimal performance. During the first phase (up to 90 min), the material from the middle vessel is redistributed between the top and bottom vessel such that the composition of the heaviest component in the top vessel and lightest component in the bottom vessel is negligible. This requires top and bottom compositions to drop during the first phase (see Figure 4(b)). These purities are subsequently recovered during the second phase. As the simultaneous approach has a smaller prediction (and thus optimization) window, it cannot exploit this vessel holdup redistribution effectively, resulting in a smaller OPI value of 17.92.

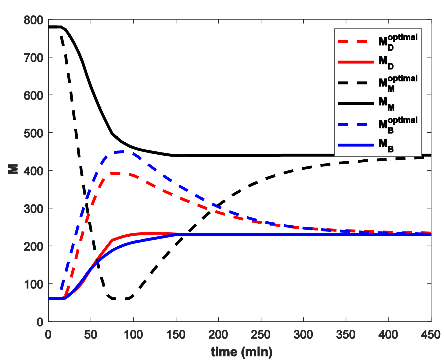


(a) Vessel holdup (M)

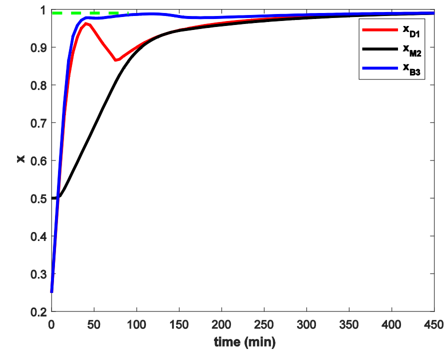


(b) Product composition

Figure 7. Dynamic response for the sequential approach with composition tracking in the presence of disturbance



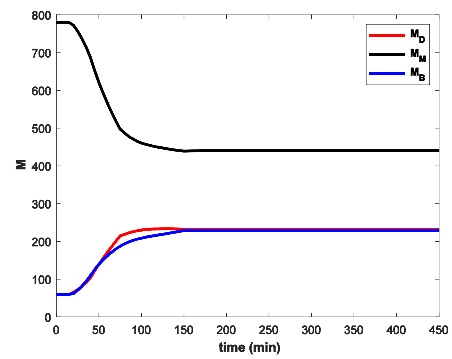
(a) Vessel holdup (M)



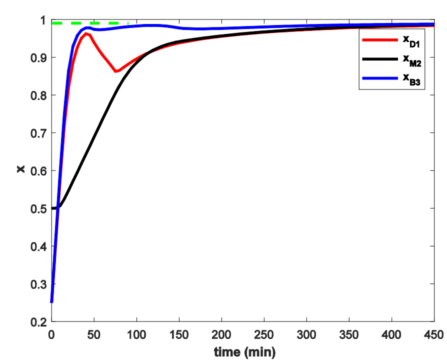
(b) Product composition

Figure 8. Dynamic response for the simultaneous approach in the absence of disturbance

In the next simulation, the performance of simultaneous approach is analysed for plant-model mismatch. The same disturbance scenario of 10% drop in the tray efficiency after 50 min of operation is considered. Figure 9 shows the corresponding vessel holdup and product composition profiles. It can be seen that the controller is still able to achieve the desired product purity at the end of the batch. Furthermore, the OPI value in this case is again 17.92. Due to runtime optimization of OPI, this controller is robust to plant-model mismatch.



(a) Vessel holdup (M)



(b) Product composition

Figure 9. Dynamic response for the simultaneous approach in the presence of disturbance

Overall, it can be concluded that, in the absence of any plant-model mismatch, all the controllers are able to meet the desired product purity. The sequential approach exhibits better performance (OPI) than the simultaneous approach due to its longer optimization horizon. However, in the presence of significant plant-model mismatch, it shows substantial decline in performance. Furthermore, the holdup tracking approach can also fail to achieve the desired end of the batch purity. On the other hand, the simultaneous approach cannot match the openloop optimal performance in terms of OPI due to its shorter optimization window. However, it is quite robust in terms of maintaining this performance and product purity even in the presence of significant plant-model mismatch.

CONCLUSION

In this paper, a comparison of two model-based control strategies, sequential (two-step) approach and simultaneous (one-step) approach, is presented for middle vessel batch distillation. The objective of optimal control is to produce products at the desired purity with optimal performance. An economic performance index (OPI) is used to evaluate the performance of MVBD column. For the case study of benzene, toluene and o-xylene separation, the proposed approaches are compared in terms of the effectiveness, overall performance and robustness to plant-model mismatch. In the absence of any disturbance, both the approaches effectively track the optimal trajectory. However, in presence of significant plant-model mismatch, the sequential approach results in substantial performance deterioration. The simultaneous approach shows robustness to plant-model mismatch, but at the cost of sub-optimal performance. Thus a trade-off between performance and robustness is observed through the sequential and simultaneous approaches.

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