Optimal operation and tracking control of vapor-recompressed batch distillation

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Abstract

Vapor recompressed batch distillation (VRBD) is an energy-integrated configuration which works on the principle of a heat pump. Operation of such a column is challenging due to unsteady, nonlinear dynamics and strong interplay between separation and energy efficiency. In this paper, a two-step approach is proposed for optimal operation and control of such a column. Initially, an openloop optimal operation policy is generated for maximization of an overall performance index using offline optimization. To this end, three performance indices are proposed to capture interplay between separation and energy efficiency. Subsequently, a model-based output feedback controller is designed to track this optimal performance trajectory. The effectiveness of the proposed approach is demonstrated using a benzene-toluene separation case study wherein it is shown that the proposed approach helps to achieve optimal operation in the presence of operational disturbances.

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Introduction

Distillation is one of the most favoured methods for separation of liquid mixtures in chemical industry. At the same time, it is one of the major consumer of energy in a manufacturing system. Application of energy integration for distillation column(s) has thus received significant attention over the last five decades, especially for continuous distillation, resulting in energy efficient configurations such as vapor recompressed distillation, multi-effect distillation, divided wall column, heat-integrated distillation (HiDiC), etc.[1] Initially, batch distillation was excluded from this exercise due to small quantum of savings.[2] With increased competition and fluctuating energy price, the design of energy-integrated batch distillation column has gained increased attention. Most of the existing energy-integrated batch distillation configurations are extensions/modifications of the corresponding continuous distillation counterparts, such as vapor recompressed batch distillation (VRBD),[3,4] multi-effect batch distillation (also known as multi-vessel batch distillation),[2,5–8] divided wall batch distillation[9] and heat-integrated batch distillation.[9,10]

Vapor recompression-based distillation uses energy available with the top vapor to vaporize liquid at the bottom of the column. This requires compressing the top vapor[3] (and thus elevate its condensation temperature above the bubble point of the bottom liquid) or flashing of the bottom liquid[11] (thereby reducing its bubble point below the condensation temperature) in order to generate favourable thermal driving force. Such thermal coupling between the stripping and rectification section of the column results in energy recycle within the column and has been shown to give rise to multi-time scale dynamics in the corresponding continuous vapor recompressed distillation column.[12] In the case of vapor-recompressed batch distillation, in addition to this energy recycle, one has to deal with the time-dependent variation of the condenser and reboiler load while operating such a column. Furthermore, it has been shown that the underlying process dynamics are typically nonlinear.[13] Previously, regulatory control of vapor recompressed batch distillation has been pursued to achieve constant distillate purity, through the manipulation of reflux flow, using a variable gain PI controller,[4] a nonlinear geometric controller[13,14] or an optimization-based controller.[13] This is augmented by a thermal driving force control system which manipulates the compressor speed via a model-based openloop (computed) controller.[11] All these approaches focus only on the separation performance during the production phase and use an arbitrary, constant product withdrawal rate. As the primary reason for the vapor-recompressed configuration is to save energy, it is essential to track/minimize energy consumption along with production maximization. However, in the existing literature, energy minimization is limited only to the startup phase (total reflux).[6,7] Lastly, for energy-integrated batch distillation columns, it has also been shown that there is a clear trade-off between quality of control and energy consumption.[6] Motivated by this, this work aims at systematically addressing the trade-off between production and energy consumption to facilitate optimal operation of a vapor-recompressed batch distillation column.

In our approach, we first define three performance indices to capture effectiveness of the VRBD system in terms of production, energy consumption or both. An openloop optimization problem is solved to obtain a trajectory of key system variables to maximize the selected performance index. Subsequently, a model-based control system is designed to track this optimal trajectory in the presence of disturbances and/or plant-model mismatch.

The rest of the paper is organized as follows. Initially, a brief overview of the VRBD system, in terms of its operating principle, operational phases, dynamic equations and control requirements, is presented. The next section focuses on the definition of performance indices and formulation of the corresponding openloop optimization problem. A model-based control system, along with a nonlinear state estimator, to track this optimal profile is designed in the following section. A case study is then presented to highlight the effectiveness of the proposed strategy.

Vapor Recompressed Batch Distillation (VRBD)

Vapor recompressed batch distillation, as shown in Figure 1, is an energy-integrated configuration based on the principle of a heat pump.[3] The top vapor is the heat source, whereas the bottom liquid is the heat sink. The negative thermal driving force necessitates use of a heat pump. The condensation temperature of the vapor leaving the top of the column is increased using the compressor. This allows us to use a combined reboiler-condenser to achieve energy integration. It is assumed that the heat transferred by the compressed vapor is less than the reboiler duty. The remaining amount of energy is provided through the auxiliary reboiler. The condensate leaving the reboiler-condenser is throttled and sent to the reflux drum. The distillate is withdrawn from the reflux drum and collected in the product tank. The overall operation of a VRBD system consists of two phases:

- Start-up phase: The column is initially operated at total reflux condition (zero product withdrawal). The vapor generation rate in the column is held constant by manipulating the required utility. This phase ends when the desired top purity is reached.

- Production phase: This phase is characterized by the withdrawal of distillate as a product. This product removal causes the purities as well as the dew/bubble point temperature of the top vapor and the bottom liquid to deviate from the start-up phase values and requires continuous intervention (through control) to achieve product withdrawal at the desired purity. Additionally, sufficient holdup needs to be maintained inside the reflux drum to facilitate product withdrawal.

For simplicity, let us consider a binary separation system with constant tray holdup and constant molar overflow assumption. The dynamics of the corresponding VRBD system is governed by the following equations.

$$\begin{aligned}
\frac{dM_D}{dt} &= V - R - D \\
\frac{dx_D}{dt} &= \frac{1}{M_D}\left[V\left(y_1 - x_D\right)\right] \\
\frac{dx_i}{dt} &= \frac{1}{M_i}\left[R\left(x_{i-1} - x_i\right) + V\left(y_{i+1} - y_i\right)\right] \\
\frac{dM_B}{dt} &= R - V \\
\frac{dx_B}{dt} &= \frac{1}{M_B}\left[R\left(x_N - x_B\right) + V\left(x_B - y_B\right)\right] \\
\frac{dM_p}{dt} &= D \\
\frac{dx_{D,avg}}{dt} &= \frac{D\left(x_D - x_{D,avg}\right)}{M_p}
\end{aligned} \tag{1}$$

Here, x and y represent mole fraction of the more volatile component in the liquid and vapor phase, respectively. M, V, R and D represent molar holdup, vapor flow rate, reflux flow rate and distillate flow rate, respectively. The subscripts D, B, i and p represent reflux drum, reboiler, i^{th} tray and product tank, respectively. The trays are numbered starting from the top. A constant thermal driving force (ΔT) is maintained between the compressed vapor temperature (T_C) and the temperature of the reboiler liquid (T_B). The unsteady operation of the VRBD system requires the compressor to operate at a variable speed to maintain constant ΔT throughout the batch.[4] The corresponding compression ratio (CR) required is estimated using the following equation.

$$CR = \left[\frac{T_C}{T_T}\right]^{\left(\frac{\mu}{\mu-1}\right)} \tag{2}$$

Here, T_T and T_C represent the uncompressed and compressed top vapor temperature, respectively and μ represents the specific heat ratio.

Remark 1 *Positive thermal driving force in a VRBD system can also be achieved by flashing the bottom liquid to reduce its bubble point.*[11] *Subsequently, the vapor generated from the combined reboiler-condenser is compressed to the column pressure. It can be noted that this configuration differs from the one discussed above only in terms of the position of the compressor (bottoms versus the distillate stream). As the control objectives, manipulated variables and economic objectives are the same, the analysis presented in this paper is applicable to this configuration as well.*

Remark 2 *In this paper, it is assumed that the reboiler load is greater than the condenser load, resulting in the requirement of the auxiliary reboiler. For some systems, the converse can be true and they would require an auxiliary condenser instead of a reboiler. By replacing auxiliary reboiler with a condenser, the analysis presented in this paper can also be applied to this case. It should be noted that the cost of reboiler duty (e.g. steam) is generally higher than the cost of condenser duty (e.g. cooling water) and thus the trade-off between production and energy consumption will have less impact than the case considered in this paper.*

Openloop Operation Policy

In this section, we develop a dynamic optimization formulation to generate optimal trajectory for key variables of the VRBD system. In order to characterize the notion of optimal operation, we define the following performance indices which capture effectiveness of the VRBD system.

1. Production Performance Index (PPI): The primary objective of a distillation system is to produce high value products which meet quality and quantity specifications. The PPI, therefore, captures the separation yield which should be maximized through optimal operation. The PPI is defined as the amount of more volatile component recovered as a fraction of the initial charge and is computed using the following equation.

$$PPI = \frac{M_p(t_f)x_{D,avg}(t_f)}{M_0 z_F} \tag{3}$$

   Here, t_f represents the end of the batch time, M_0 represents the initial molar charge with z_F as the mole fraction of the more volatile component in the feed.

2. Energetic Performance Index (EPI): Improvement of energetic performance of batch distillation is the primary reason for installing a VRBD system. It is therefore important to track energy savings offered by the VRBD column as compared to an equivalent (with the same composition profile) conventional batch distillation (CBD) column. The EPI, therefore, captures the energy efficiency of the separation. It is defined as the total energy saved by using the VRBD configuration as a fraction of the energy consumed in an equivalent CBD column. It is

computed using the following equation.

$$EPI = \frac{Q_{total,CBD} - Q_{total,VRBD}}{Q_{total,CBD}} \tag{4}$$

Here, Q_{total} represents the total energy consumed during the distillation operation. For the CBD column, this corresponds to the total reboiler load (assuming negligible condensation cost). For the VRBD system, there are two significant energy inputs; auxiliary reboiler duty (Q_{aux}) and the compressor power (W). As the cost of thermal energy is different than the electrical energy, the overall energy consumed in a VRBD system is computed by the following equation.

$$Q_{overall} = Q_{aux} + \phi W \tag{5}$$

Here, ϕ (> 1) represents the cost factor for conversion of electrical energy into equivalent thermal duty. $Q_{total,VRBD}$ is then the integration of $Q_{overall}$ over the batch time.

3. Overall Performance Index (OPI): It can be noted that the PPI focuses on production without accounting for utility consumption. On the other hand, the EPI targets energy savings without considering overall production. It is therefore logical to define a performance index which combines both these aspects and computes the overall efficiency of the operation. To this end, OPI is defined as the amount of product collected per unit energy consumption. It is computed using the following equation.

$$OPI = \frac{M_p(t_f)x_{D,avg}(t_f)}{Q_{total,VRBD}} \tag{6}$$

Remark 3 *These definitions of performance indices can be easily extended for multi-component separation. In multi-component separation, the bottom residue obtained after the end of the production phase is subjected to a new start-up phase (with or without addition of an intermediate feed).*[15] *When the desired product purity for the second cut is achieved, the second production phase is started. For multiple product cuts, this sequence of start-up and production phase is repeated multiple times. In this context, the PPI, EPI and OPI definitions are modified as follows:*

$$
\begin{aligned}
PPI_i &= \frac{D_{total,i} x_{D,avg,i}(t_{f,i})}{M_0 z_{F,i}} \\
EPI_i &= \frac{Q_{total,CBD,i} - Q_{total,VRBD,i}}{Q_{total,CBD,i}} \\
OPI_i &= \frac{D_{total,i} x_{D,avg,i}(t_{f,i})}{Q_{total,VRBD,i}} \qquad (7)
\end{aligned}
$$

Here, PPI_i, EPI_i and OPI_i are the PPI, EPI and OPI index for the i^{th} product, $D_{total,i}$ is the total amount of distillate collected and $t_{f,i}$ is the production phase duration for the i^{th} product. $Q_{total,CBD,i}$ and $Q_{total,VRBD,i}$ represent the total energy consumptions during the i^{th} production phase.

Formulation of openloop optimization problem

The operation of VRBD column is inherently dynamic and therefore it is essential to generate optimal trajectory of process variables while taking the batch from the feed conditions to the final desired state. Thus a dynamic optimization problem needs to be formulated which can be solved offline to generate such a trajectory. The following are the components of the corresponding optimization problem.

Objective function: The optimal operating policy can be generated to maximize production, minimize energy consumption or a combination thereof. To this end, the performance indices defined earlier can be used as an objective function. Thus three objective functions can be considered, namely, maximization of PPI, maximization of EPI or maximization of OPI.

Decision variables: These include the product withdrawal rate (D) during the production phase, reflux flow (R) and auxiliary reboiler duty (Q_{aux}). For the optimization formulation, deviations of these variables from their values at the end of the start-up phase are considered as the decision variables. A piece-wise constant input policy is considered.

Constraints: The ODE system (1) governing the dynamic evolution of the VRBD column represents the main constraint. The ODEs are discretized using a suitable numerical scheme (e.g. implicit Euler, Runge Kutta, etc.). A terminal constraint is put on $x_{D,avg}$ to achieve the desired final product purity. A trajectory constraint is put on the reflux drum holdup (M_D) to maintain sufficient inventory throughout the operation. Upper and lower limit constraints are put on decision variables as well as mole fractions (x_i) at each stage. In order to ensure feasible transition, input change at any time step is also constrained below a maximum value.

Remark 4 *The overall performance index (OPI) can be easily converted into an economic performance index. It can be redefined as the value of the product obtained per unit utility cost. It can be argued that the terminal product purity constraint will be active in the OPI maximization problem solution. Based on this, as shown in Eq. (8), the optimal economic performance index will be approximately a scaler multiple of the OPI defined earlier. The maximization of OPI is thus equivalent to the corresponding* *optimization of the economic performance index.*

$$
\begin{aligned}
OPI_{economic} &= \frac{P_{product} M_p(t_f)}{P_{utility} Q_{total,VRBD}} \\
&= \frac{P_{product}}{P_{utility}} OPI \frac{1}{x_{D,avg}(t_f)} \\
&\approx \frac{P_{product}}{P_{utility} x_{D,avg,desired}} OPI
\end{aligned} \tag{8}
$$

Remark 5 *Out of the three performance indices, only EPI can be computed for the start-up phase. Also, one decision variable, D, is inactive during the start-up phase. Considering this, this paper focusses on generating the optimal operation policy only for the production phase. To compute optimal policy during the start-up phase, one can consider modifying the existing approaches for multi-vessel batch distillation[6, 7] towards VRBD. Alternatively, one can also solve EPI maximization problem with R and Q_{aux} as the decision variables.*

Model-based Control

The optimal operation policy generated in the previous section can be directly implemented to the VRBD column, provided there are no external disturbances or plant-model mismatch. During actual operation, both these factors would come into play and thus, there is a need for feedback control to satisfy process constraints and maintain operational optimality. To this end, a model-based controller is designed in this section. The objective of this controller is to track the optimal operation policy in the presence of disturbances and plant-model mismatch. The key variable to be tracked is the average distillate purity ($x_{D,avg}$). In order to facilitate product withdrawal and product purity control through reflux, reflux drum holdup (M_D)

is also tracked along its optimal trajectory. These control objectives can be achieved through the manipulation of reflux flow rate (R), distillate withdrawal rate (D) and auxiliary reboiler duty (Q_{aux}).

Figure 2 depicts the schematic of the resulting control and optimization system. The batch performance specs (e.g. desired product purity $x_{D,avg,desired}$, minimum reflux drum holdup $M_{D,min}$, etc.) are fed to the offline optimizer to generate optimal operation profile. Out of these, $x_{D,avg}$ and M_D profile are used as set points for the corresponding model-based state-feedback controller, whereas D profile is directly fed to the process. The controller generates the required values of R and Q_{aux} to achieve the targets. As most of the state variables are compositions and thus difficult to measure online at a fast rate, a state estimator is incorporated to generate fast estimates of these compositions. These estimates are used in the state-feedback controller. The design of the state estimator as well as the model-based controller is presented below.

Remark 6 *Instead of directly feeding D profile to the column, it can also be used as a manipulated variable in the controller, resulting in a 2 output-3 input controller. In this paper, we have considered a model-based controller which requires equal number of controlled and manipulated variables. Therefore we have an option of directly feeding one of the manipulated inputs.*

D has direct impact on PPI and thus the selected strategy of directly feeding D profile helps achieve closed-loop PPI values closer to the openloop optima. Alternatively, one can also direct-feed Q_{aux} profile and use D and R as manipulated variables. This setup will achieve closed-loop EPI values closer to the openloop optima.

State estimation

Continuous knowledge of composition throughout the column plays an important role in the effective implementation of the optimal operation profile during batch operation.[16,17] As direct composition measurement is costly and often delayed, on-line state estimator is typically implemented to get the real-time composition estimates from fast, easily available measurements. Extended Kalman Filter (EKF) is one of the most favoured estimators to provide reliable state estimates in the presence of plant-model mismatch and process & measurement noise.[18] Previously, it has been recommended, for robust convergence of estimates, that at least $(N_C + 2)$ measurements be used.[19] Here, N_C is the number of components present in the mixture. To this end, temperatures on stages 2, 4 and 10 (T_2, T_4 and T_{10}) along with holdup of reboiler (M_B) and reflux drum (M_D) are considered as available measurements.

The process model given by Eq. (1) is discretized with a sampling time of T_s. Additionally, it is considered that the temperature at any stage is given by the corresponding bubble point and the corresponding equations are included in the model.

State-feedback controller

The dynamics of VRBD column is nonlinear[13] and therefore a nonlinear model-based controller is designed. Globally linearizing controller (GLC) is an efficient and one of the most widely used nonlinear control techniques of feedback linearization.[20] In GLC, a nonlinear state-feedback law is synthesized to linearize the input-output map. For the VRBD column, the controlled variables are $x_{D,avg}$ and M_D. The manipulated variables are Q_{aux} and R. For this 2×2 control system, the characteristic matrix (representative of the nonlinear process gain matrix) becomes singular during operation. Due to this, the controller becomes ill-conditioned. To this end, instead of $x_{D,avg}$, top tray purity (x_1) is used as a controlled variable. Also, the reflux drum holdup dynamics are linear and need not be tracked tightly. So, it is controlled using a simple proportional controller to simplify controller design. In this setting, the relative degree between the input-output pair is one. Accordingly, the GLC is designed to request the following closed-loop response:

$$\beta \frac{dx_1}{dt} + x_1 = v$$

The corresponding nonlinear state-feedback law is computed as

$$\begin{bmatrix} R \\ Q_{aux} \end{bmatrix} = \begin{bmatrix} \beta \mathcal{L}_g x_1 & 0 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} v - x_1 - \beta \mathcal{L}_f x_1 \\ Q_{aux,nom} + K_{C,2}\left(M_{D,set} - M_D\right) \end{bmatrix} \tag{9}$$

where $\mathcal{L}$ represents a *Lie* derivative, and f and g are vector fields corresponding to Eq. (1) when written in the following vector form.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u} \tag{10}$$

In order to achieve an offset-free response in $x_{D,avg}$ in the presence of disturbances and plant-model mismatch, the following external integral action is added in the GLC control scheme.

$$v = x_{1,set} + K_{C,1}\left(x_{D,avg,set} - x_{D,avg}\right) + \frac{K_{C,1}}{\beta} \int_0^t (x_{D,avg,set} - x_{D,avg}) d\tau \tag{11}$$

This control system has β and K_{Ci} as the controller tuning parameters.

Case Study

Let us now consider a case study of benzene/toluene separation in a VRBD column, depicted in Figure 1, to illustrate the operational framework developed earlier. The column has a total of 8 trays. For simplicity, the pressure drop in the column is assumed to be negligible. The relative volatility, tray holds up, specific heat capacity and liquid flow rate from tray to tray are assumed to be constant across the column. The VRBD column reaches the desired operating state in 320 min and the start-up phase ends. The various design parameters as well as the values of key variables at the end of the start-up phase are given in Table 1.

Let us first generate openloop operation policy for this VRBD column. The openloop optimization problem formulated earlier is solved separately for the maximization of PPI, EPI and OPI. The corresponding nonlinear programming problem (NLP) problem is solved using CasADi.[21] For each of these cases, the optimal solution is obtained for various values of product purity specification and a fixed production phase of 2000 min. The details of the optimal solutions are included in Table 2.

It can be noted that, as the desired product purity increases, the PPI decreases. For some of the cases, especially with high PPI, negative EPI is observed. This means the effective energy demand of the VRBD column is more than the corresponding non-integrated column, thereby defeating the purpose of using a VRBD column. Even for the other cases, there isn't any significant reduction in energy consumption due to energy integration (maximum of 2.6%). This clearly shows that simply focusing on production maximization (through PPI) is not a rational approach for an energy-integrated configuration like VRBD.

Maximization of EPI leads to around 7% reduction in the net energy consumption, demonstrating energy efficiency of the VRBD scheme. However, it can be seen that this comes at the cost of reduced production (29-65% of the maximum possible production). This clearly indicates the need for a trade-off between production and energy consumption.

For the case of OPI maximization, significant production as well as energy savings are obtained for all the product purity specifications. For example, for product purity of 0.985, PPI maximization resulted in minimum EPI, whereas EPI maximization gave the minimum PPI. The OPI maximization problem provided a decent trade-off by achieving 76% of the maximum production (PPI) and 79% of the maximum energy savings (EPI). This clearly highlights the importance of OPI in capturing the overall effectiveness of VRBD operation. Therefore, for the subsequent closed-loop studies, maximum OPI trajectories are tracked.

Table 3 lists the parameters used for the extended Kalman filter. It is considered that the initial condition for the estimates ($\hat{x}_0$) is 97% of the actual state value. The comparison of the actual and estimated states is depicted in Figure 3. It can be seen that the state estimates quickly converge to the real states even though the initial conditions are significantly different.

Let us now consider closed-loop performance of the VRBD column under OPI maximization strategy. The various controller tuning parameters are listed in Table 4. Figure 4 depicts the response of the closed-loop system for the product purity of 0.925 and a production phase of 1150 min. For this case, the openloop PPI, EPI and OPI are 0.36, 0.13 and 14.30, respectively. It can be seen that the controller is able to track the optimal trajectories of the key variables and the obtained performance indices are in agreement with the openloop values. As a disturbance scenario, we considered that after 100 min into the production phase, tray efficiency for all the trays in the column dropped by 5% due to an undetected fault. The corresponding closed-loop response is depicted in Figure 5. It can be seen that the proposed control structure is able to handle such a large unaccounted disturbance, resulting in performance indices which are within 2.5% of the openloop values (PPI = 0.36, EPI = 0.13 and OPI = 13.95).

Next, we considered operation of the VRBD column at a higher purity point. Figure 6 depicts the closed-loop response for $x_{D,avg}$ of 0.985 and a production phase of 750 min. In the absence of any disturbance, the control system is able to effectively track the optimal trajectory. We also considered a disturbance scenario wherein the tray efficiency for all the trays falls by 2%. The corresponding response of the system is depicted in Figure 7. It can be seen that the controller is able to handle this disturbance, however, with certain instances of the reflux drum level falling below the lower limit (0.1 kmol). Any larger disturbance cannot be handled as the required reflux rate for this high purity operation completely drains the reflux drum.

Lastly, we solved the OPI maximization problem for various values of production phase duration to obtain the optimal batch time. For this case, the OPI definition is slightly modified to include energy consumption during the start-up phase as well. The corresponding variation of the performance indices as a function of the production phase duration, for various product purity specifications, is depicted in Figure 8. It can be seen that there is no clear optima for PPI or EPI with respect to the production phase duration. On the other hand, OPI shows a clear maxima for each product purity specification. The optimal value of OPI decreases with an increase in the product purity specification. It is interesting to note that the optima is relatively flat, indicating a wide range of optimal production phase duration.

Concluding Remarks

In this paper, we have focused on the operational aspects of vapor-recompressed batch distillation (VRBD) configuration. To evaluate effectiveness of its operation, we defined three performance indices in terms of separation yield and energy saving. The optimal operation problem is decomposed into openloop trajectory optimization and closed-loop tracking of the optimal profile. Trajectory optimization is pursued for maximization of each of the performance indices in the presence of operating constraints. Subsequently a model-based controller is designed for tracking this optimal profile. Through a case study of benzene/toluene separation in a VRBD column, it is shown that OPI is an effective performance index to capture trade-off between production and energy consumption. An input-output linearizing controller, along with an EKF-based estimator, performs well to track this optimal trajectory. This configuration achieves close to optimal indices even in the presence of significant disturbances. Lastly, it has been shown that OPI maximization can also be used to obtain optimal batch time.

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Figures

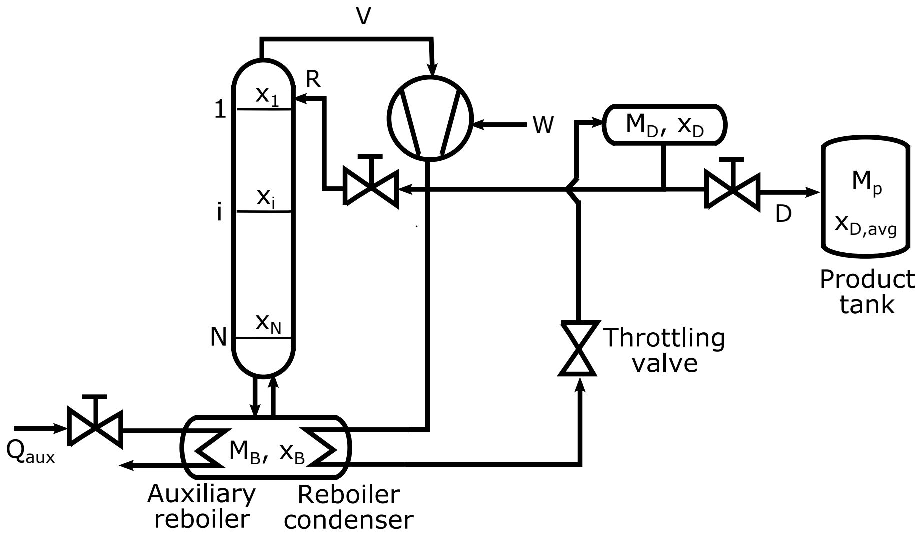


Figure 1: Schematic of vapor-recompressed batch distillation

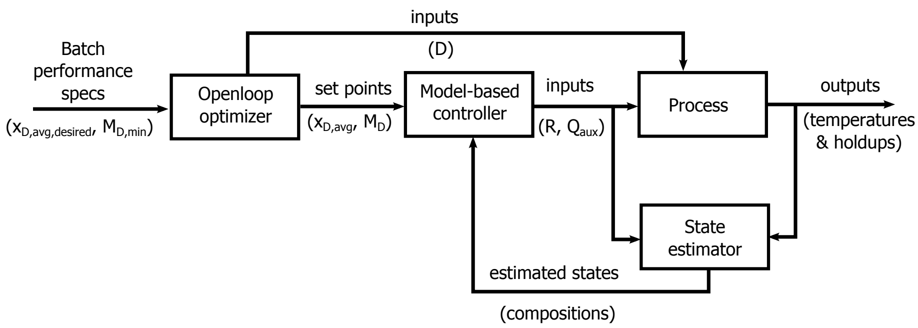
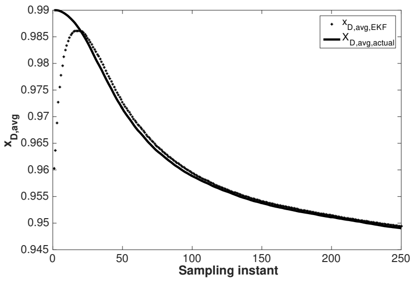
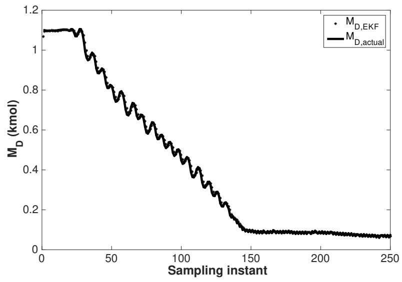


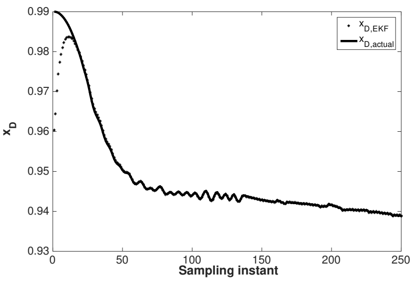
Figure 2: Schematic of the control and optimization system



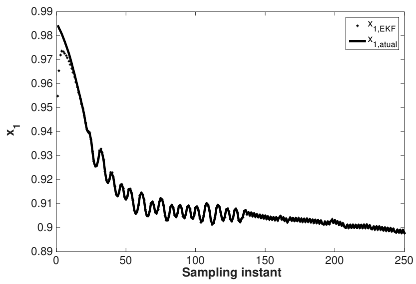
(a) $x_{D,avg}$



(b) M_D

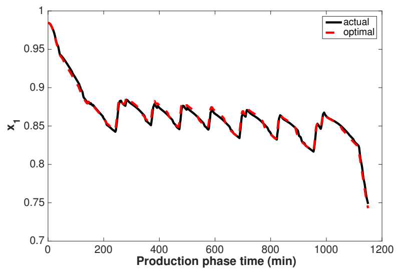


(c) x_D

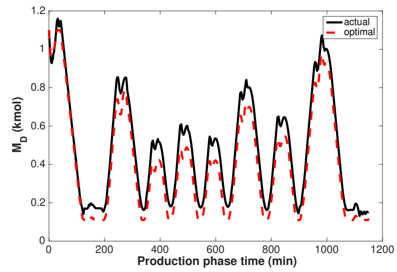


(d) x_1

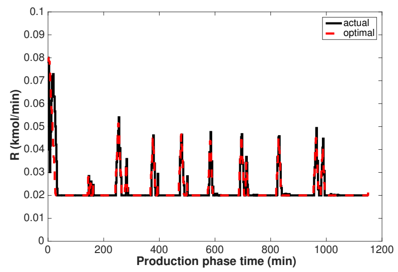
Figure 3: Comparison of actual and estimated states



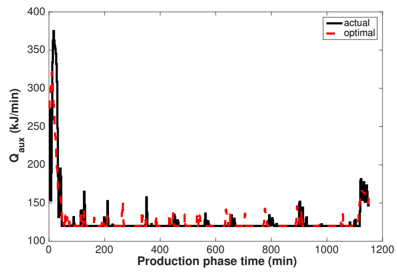
(a) x_1



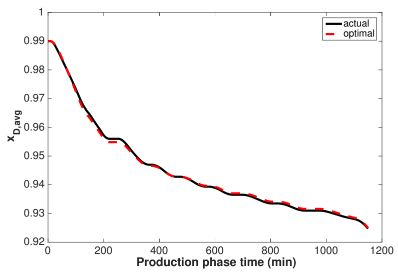
(b) M_D



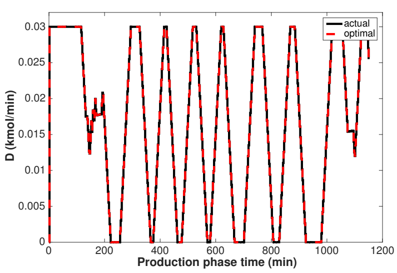
(c) R



(d) Q_{aux}

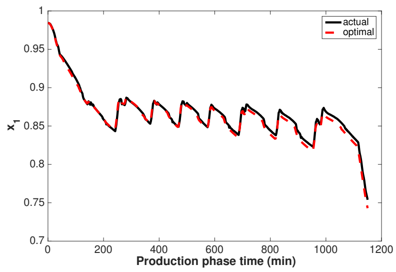


(e) $x_{D,avg}$

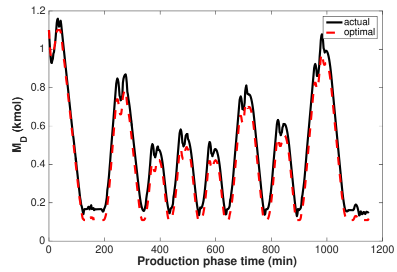


(f) D

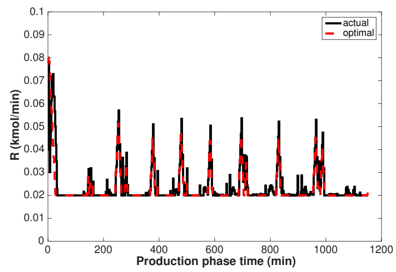
Figure 4: Closed-loop performance of the VRBD system for OPI maximization with product purity of 0.925 (without disturbance)



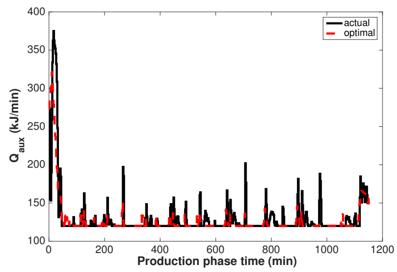
(a) x_1



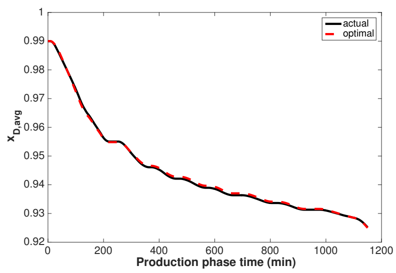
(b) M_D



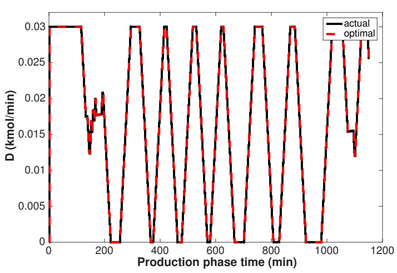
(c) R



(d) Q_{aux}

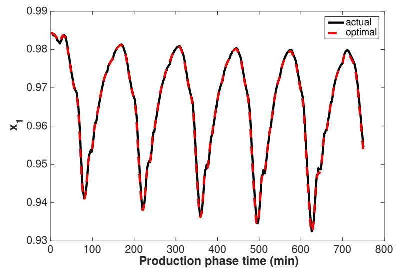


(e) $x_{D,avg}$

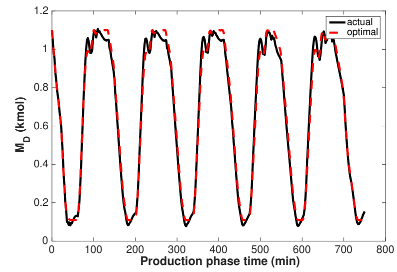


(f) D

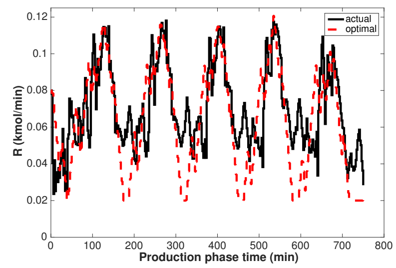
Figure 5: Closed-loop performance of the VRBD system for OPI maximization with product purity of 0.925 (with -5% disturbance)



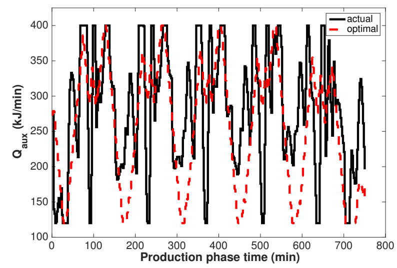
(a) x_1



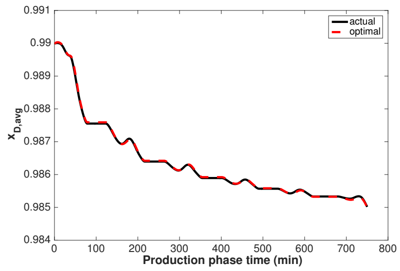
(b) M_D



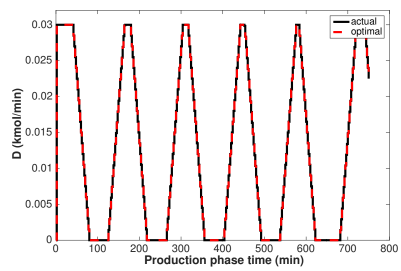
(c) R



(d) Q_{aux}

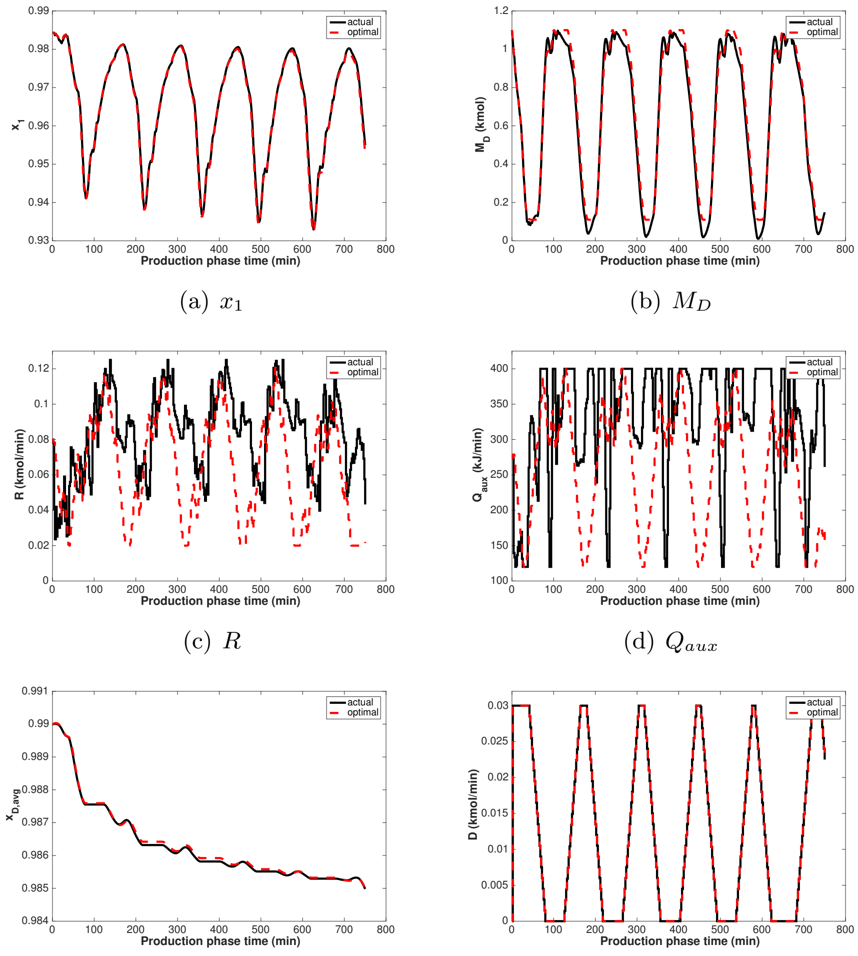


(e) $x_{D,avg}$



(f) D

Figure 6: Closed-loop performance of the VRBD system for OPI maximization with product purity of 0.985 (without disturbance)

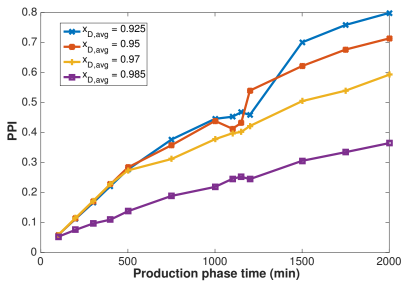


(a) x_1 (b) M_D

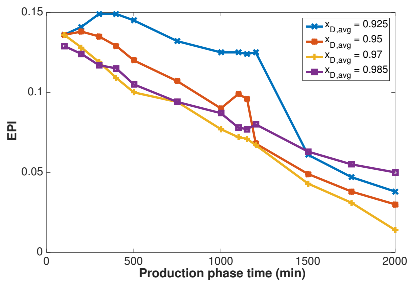
(c) R (d) Q_{aux}

(e) $x_{D,avg}$ (f) D

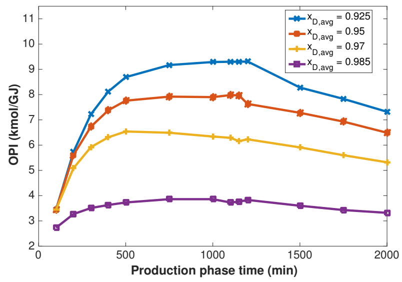
Figure 7: Closed-loop performance of the VRBD system for OPI maximization with product purity of 0.985 (with -2% disturbance)



(a) PPI



(b) EPI



(c) OPI

Figure 8: Variation of performance index as a function of the production phase duration

Tables

Table 1: VRBD column details for benzene/toluene case study

Variable	Value
Number of stages	8
Total fresh feed, M_B	100 kmol
Feed composition	0.5/0.5
Tray holdup, M_i	0.25 kmol
Reflux drum holdup, M_D	1.1 kmol
Distillate composition, x_D	0.99
Tray efficiency	64.5 %
Reflux rate, R_{ss}	0.08 kmol/min
Auxiliary duty, $Q_{aux,ss}$	273.5 kJ/min
Total reboiler duty, $Q_{Reboiler}$	2500 kJ/min
Cost factor, ϕ	3

Table 2: Results for openloop optimization

$x_{D,avg}$	D_{total} (kmol)	$Q_{total,VRBD}$ (GJ)	PPI	EPI	OPI (kmol/GJ)
		PPI maximization			
0.925	45.92	5.3958	0.85	-0.035	7.87
0.935	44.30	5.4146	0.83	-0.042	7.65
0.95	40.55	5.3691	0.77	-0.043	7.17
0.965	34.69	5.297	0.67	-0.028	6.32
0.985	19.32	4.9297	0.38	0.026	3.86
		EPI maximization			
0.925	29.55	4.6736	0.55	0.075	5.85
0.935	25.93	4.6739	0.48	0.074	5.19
0.95	19.56	4.6741	0.37	0.074	3.98
0.965	13.41	4.6741	0.26	0.067	2.77
0.985	5.61	4.6767	0.11	0.073	1.18
		OPI maximization			
0.925	36.09	3.2455	0.67	0.067	10.29
0.935	34.26	3.2519	0.64	0.060	9.85
0.95	30.85	3.2672	0.59	0.053	8.97
0.965	25.51	3.1289	0.49	0.050	7.87
0.985	14.63	3.2832	0.29	0.058	4.39

Table 3: Parameters for extended Kalman filter

Parameter	Value
Q	$10^{-8}\mathrm{diag}(0.01, 1, 1, 1, 1, 1, 1, 1, 1, 0.01, 1000, 100, 0.01, 0.01)$
R	$10^{-4}\ \mathrm{diag}(1, 1, 1, 1, 0.01)$
P_0	$10^{-6}\mathrm{diag}(5, 5, 5, 5, 5, 5, 5, 5, 5, 0.05, 5, 5, 5, 5)$

Table 4: Controller tuning parameters

Parameter	Value
β	1 min
$K_{C,1}$	0.02
$K_{C,2}$	3000 J/mol/min