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Model-based Control of Vapor-recompressed Batch Distillation Column ⋆

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Abstract: This article provides a comparison of control strategies for an economically attractive vapor-recompressed batch distillation (VRBD) column. A VRBD column exhibits nonlinear dynamics with strong inter-stream interactions due to energy-integration, which can give rise to difficulties in controlling the operation using traditional linear controllers. In this paper, we propose and compare model-based control strategies such as linear quadratic regulator (LQR), linear model predictive control (LMPC) and Globally linearizing controller (GLC) for a VRBD column to achieve desired distillate purity with minimum energy consumption. The effectiveness of these control strategies is illustrated using a simulation case study of benzene/toluene separation in a VRBD column.

Keywords: Energy-integration, heat pump, batch distillation, model-based control, input/output linearization, linear quadratic regulator, model predictive control.

1. INTRODUCTION

As the chemical and allied industries are growing at a faster rate and non-renewable energy resources are depleting day by day, it is necessary to perform most of the industrial operations in an energy saver mode. One of the ways to achieve this is to thermally integrate process streams and get economic benefits. Such an integration involves identification of energy sources and sinks within a system and establishing energy transfer between them to reduce the use of external utilities.

Due to operational flexibility and repeatability, batch processes are getting attention of researchers in recent years (Fernández et al., 2012). It is economically attractive to incorporate energy integration in batch processes, but strong coupling between process streams resulting from such integration gives rise to hybrid (continuous + discrete) two-time scale dynamics (Jogwar and Daoutidis, 2015). In such a case, control system design to achieve desired performance of the process is a challenging task.

Distillation is one of the most widely used separation processes with high energy consumption and low thermodynamic efficiency. The disadvantage of low thermodynamic efficiency of distillation can be overcome by incorporating energy-integration. Numerous thermally coupled configurations and control strategies have been developed for continuous distillation column to improve economics and lower energy consumption (see Jogwar and Daoutidis (2010) for a review), whereas limited literature is available on energy-integrated batch distillation (Babu and Jana, 2014).

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Vapor-recompressed Batch Distillation (VRBD), as depicted in Figure 1, is one such energy-integrated configuration of batch distillation (Babu and Jana, 2014). As the product is withdrawn from the VRBD column, similar to conventional batch distillation, the product purity starts to drop from the desired value. In order to maintain the product purity, a feedback control system is needed. The major operational challenge comes from the fact that the deviations in product purity disturb the thermal balance between the heat source and sink, and can easily destabilize the system. In order to address this control problem in a systematic manner, we propose to use model-based control configurations to achieve product purity control while ensuring stability and optimality of operation.

In this paper, several model-based control strategies are explored for efficient operation of a VRBD column. Firstly, linear quadratic regulator (LQR) which is the simplest form of optimal control is considered. Linear model predictive controller (LMPC) is designed to systematically handle operating constraints. Lastly, a nonlinear control scheme is designed with the help of input/output linearization to account for nonlinearity in the production phase.

The rest of the paper is organized as follows. Section 2 describes the configuration and operating principle of VRBD. Section 3 presents design of various model-based control strategies for a VRBD column. Closed-loop performances of the VRBD column with the above control strategies are presented in Section 4 for a simulation case study of benzene-toluene separation and concluding remarks are drawn in Section 5.

2. VAPOR RECOMPRESSED BATCH DISTILLATION

Vapor-recompressed batch distillation is an energy-integrated configuration which works on the principle of

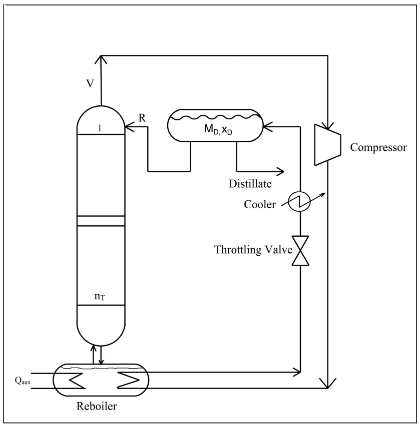

Fig. 1. Vapor-recompressed batch distillation

a heat pump. Figure 1 shows a schematic configuration of a VRBD column. The overhead vapor from the column acts as a heat source and the reboiler liquid acts as a heat sink. Note that the heat source is colder than the heat sink which is thermodynamically infeasible. To ensure feasibility of heat transfer, the top vapor is compressed in a compressor to raise its condensation temperature. A thermal driving force (ΔT) is to be maintained between the temperature of the compressed top vapor (T_C) and the reboiler liquid (T_B) throughout the batch. As the operation of a VRBD column is dynamic, the top tray temperature (T_T) and the reboiler temperature vary with time. The compressor therefore operates at a variable speed to maintain constant ΔT throughout the batch operation. The corresponding compression ratio (CR) required is estimated as:

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

where μ is the specific heat ratio. As the thermal energy associated with the condensing vapor may not always be sufficient to generate the required amount of vapor, an auxiliary reboiler is installed to cover for any deficit amount of heating duty.

The overall operation of VRBD consists of two phases:

- Start-up phase: At first, the column is operated at total reflux conditions and no product is withdrawn. The start-up phase ends when a steady state with the desired product purity is reached.
- Production phase: This phase starts with the withdrawal of distillate as a product. As mentioned earlier, this causes the purities as well as the dew/bubble point temperature of the top vapor and the reboiler liquid to deviate from the start-up phase values, requiring continuous intervention (through control) to achieve sustained product withdrawal at the desired purity. The production phase ends when either the average distillate purity ($x_{D,avg}$) or the reflux drum holdup (M_D) falls below its minimum value ($x_{D,avg,min}$ or $M_{D,min}$, respectively).

3. MODEL-BASED CONTROL STRATEGIES

The primary control objective of this system is to maintain $x_{D,avg}$ above the desired value. This is accomplished by regulating the instantaneous distillate purity (x_D).

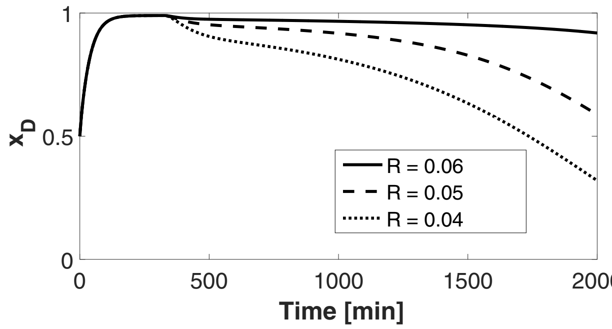

Fig. 2. Open-loop dynamics of the VRBD column for step changes in the reflux rate

Additionally, there is a need to maintain sufficient reflux drum holdup. Available manipulated inputs are the reflux rate (R) and the auxiliary reboiler duty (Q_{aux}). In order to investigate the dynamic properties of the VRBD column, we performed open loop simulations in the production phase. Step changes are given to the reflux rate and the corresponding response of the distillate purity is depicted in figure 2. It can be seen that the relationship between the reflux rate (one of the key manipulated inputs) and the product purity (the primary controlled variable) is nonlinear. Furthermore, the use of Q_{aux} as a manipulated input necessitates that the overall energy consumption of the system be optimized otherwise the primary objective of energy integration is compromised. This motivated us to explore control strategies beyond conventional PID control. In what follows, we develop several model-based control strategies to achieve these operational objectives.

3.1 Linear Quadratic Regulator (LQR)

As there is a requirement of optimal use of one of the manipulated inputs, we start with LQR, the simplest of the optimal controllers. The original nonlinear dynamic system is linearized around the steady state obtained at the end of the startup phase and discretized with a sampling time of 30 s. This results in the following discrete state-space representation of the system.

$$\begin{aligned} \mathbf{x}_{k+1} &= \boldsymbol{\phi}\mathbf{x}_k + \boldsymbol{\gamma}\mathbf{u}_k \\ \mathbf{y}_k &= \mathbf{C}\mathbf{x}_k \end{aligned} \tag{2}$$

where the states $\mathbf{x}$, inputs $\mathbf{u}$ and the outputs $\mathbf{y}$ represent deviations from the steady state. For this system, a state feedback law of the form

$$\mathbf{u}_k = -\mathbf{K}\mathbf{x}_k \tag{3}$$

can be obtained (Kumar and Jerome, 2013) to minimize a performance index J defined as:

$$J = \int_0^\infty \left(\mathbf{x}^T\mathbf{Q}\mathbf{x} + \mathbf{u}^T\mathbf{R}\mathbf{u}\right) dt \tag{4}$$

The two tuning parameters $\mathbf{Q}$ and $\mathbf{R}$ are adjusted so as to balance control performance and energy utilization.

3.2 Linear Model Predictive Control (LMPC)

The LQR indirectly penalizes excessive use of auxiliary reboiler duty. Linear MPC scheme is therefore designed to handle input constraints in a systematic way. Even though the input/output relationship is nonlinear, we explore the potential of linear MPC as it is shown to yield acceptable results even for nonlinear processes (Darby and Nikolaou, 2012). The discrete-time state space model in Eq. (2) developed earlier is used for the controller design. For this LMPC, the following objective function is considered:

$$J = \sum_{i=1}^{N_p} \left((\mathbf{y}_{set} - \mathbf{y}_i)\mathbf{W_y}(\mathbf{y}_{set} - \mathbf{y}_i)^T + \mathbf{u}_i \mathbf{W_u} \mathbf{u}_i^T \right) + \frac{\alpha_1}{(x_{D,avg} - x_{D,avg,min})} + \frac{\alpha_2}{(M_D - M_{D,min})} \tag{5}$$

alongwith the following operating constraints:

$$Q_{aux} \leq Q_{aux,max}$$
$$R \leq R_{max}$$

The last two terms of the objective function in Eq. (5) act as soft constraints to maintain the average distillate purity and reflux drum holdup above their critical values. The process behavior is predicted over the prediction horizon of $N_p = 40$ and control horizon of $N_c = 5$ is used. Optimal inputs are calculated by solving a constrained optimization problem and the first control move is implemented (Garcia et al., 1989).

3.3 Globally Linearizing Control (GLC)

The previous two control schemes used an approximate linearized model of the VRBD column which is valid only in the neighborhood of the considered steady state. Let us now design a controller based on the description of the underlying nonlinear dynamics. Globally Linearizing Control is an efficient and one of the most widely used nonlinear control techniques of feedback linearization (Kravaris and Kantor, 1990). Here, a nonlinear state feedback law is synthesized to linearize the input-output map. We considered top tray purity x_1 as the controlled variable as this is equivalent to controlling the distillate purity for a complete condenser ($x_D = y_1(x_1)$). For a 2×2 GLC controller with x_1 and M_D as outputs and R and Q_{aux} as inputs, the characteristic matrix is singular and the design of GLC controller is tricky (Soroush and Kravaris, 1994). In order to simplify controller design, we consider a GLC controller with x_1 and R as output and input, respectively. The corresponding input-output relative degree is 1. The GLC controller would achieve the following closed-loop response

$$\beta_{11}\frac{dx_1}{dt} + \beta_{10}x_1 = v = \beta_{10}x_{1,set} \tag{6}$$

using the following nonlinear state feedback law

$$u = \frac{v - \beta_{11}\mathcal{L}_f h(x) - \beta_{10}x_1}{\beta_{11}\mathcal{L}_g h(x)}$$

with

$$\mathcal{L}_g h(x) = \frac{x_D - x_1}{M}$$
$$\mathcal{L}_f h(x) = \frac{V(y_2 - y_1)}{M}$$

To further simplify the controller implementation, we approximate the instantaneous vapor flow by the steady state vapor flow ($V = V_{ss}$). This approximation results in plant-model mismatch. In order to achieve offset-free response, the following external integral action is added in the GLC control scheme.

$$v = \beta_{10}x_{1,set} + K_{C0}(x_{1,set} - x_1) + \frac{K_{C0}}{\tau_0}\int_0^t (x_{1,set} - x_1)\, dt$$

The other objective of controlling the reflux drum hold-up by manipulating auxiliary reboiler duty is achieved using a PI controller:

$$Q_{aux} = Q_{aux,nom} + K_{C1}(M_{D,set} - M_D) + \frac{K_{C1}}{\tau_1}\int_0^t (M_{D,set} - M_D)\, dt \tag{7}$$

3.4 Multi-loop PI controller

Lastly, we also compare the effectiveness of these proposed optimal and nonlinear model-based control strategies with two conventional PI controllers. Here, the reflux rate and the auxiliary reboiler duty are manipulated as:

$$R = R_{nom} + K_{C2}(x_{1,set} - x_1) + \frac{K_{C2}}{\tau_2}\int_0^t (x_{1,set} - x_1)dt$$
$$Q_{aux} = Q_{aux,nom} + K_{C3}(M_{D,set} - M_D) + \frac{K_{C3}}{\tau_3}\int_0^t \left(M_{D,set} - M_D\right) dt \tag{8}$$

In order to compare these control strategies, we define two performance indices. Specifically,

- Production Performance Index (PPI): This index captures separation yield and is defined as the total distillate collected as a fraction of the total product present in the feed.
$$PPI = \frac{D_{total}}{M_0 z_F} \tag{9}$$
where D_{total} is the total distillate collected, M_0 is the total charge in the reboiler and z_F is the feed composition.
- Energetic Performance Index (EPI): This index captures the energy efficiency of the operation and is defined as the amount of product collected per unit energy consumption.
$$EPI = \frac{D_{total}}{Q_{aux,total}} \tag{10}$$
where $Q_{aux,total}$ is the total auxiliary reboiler duty used for separation.

4. SIMULATION CASE STUDY

Let us now consider a case study of benzene/toluene separation in a VRBD column. This VRBD column has total 8 trays. For simplicity, pressure drop in the column is assumed to be negligible. Constant tray holdup (M) is considered and Hildebrand model is used to predict the vapor-liquid equilibrium. We also assume constant specific heats and liquid flow rate from tray to tray. The nominal operating information of this system is given in Table 1.

It is considered that the product is withdrawn at a rate of 0.02 kmol/min in the production phase only if the distillate purity is above a threshold value (0.985). In the first simulation, we implemented the LQR-based state feedback

Table 1. VRBD column specifications

Parameter	Value
Number of stages	8
Total fresh feed M_0	100 kmol
Feed composition	0.5
Tray holdup	0.25 kmol
Reflux drum holdup	1.1 kmol
Distillate composition (x_D)	0.99
Auxiliary duty ($Q_{aux,nom}$)	273.5 kJ/min
Tray efficiency	59.5%

Table 2. Comparison of controller performance

Controller	$x_{D,avg}$	Production phase [min]	PPI	EPI [kmol/GJ]
LQR	0.985	2750	0.3276	19.07
LMPC	0.985	2760	0.3372	21.46
GLC	0.985	3450	0.3572	17.14
PI	0.985	4430	0.3836	12.38

law of Eq. (3) and the corresponding responses are shown in figure 3. It can be seen that the auxiliary heat duty given by the controller is just sufficient to maintain the reflux ratio, and thus the drum hold-up, during product withdrawal by increasing vapor generation in the column. As no constraint is inserted on minimum product purity, the closed-loop system gives a PPI of 0.3276 and an EPI of 19.07 kmol/GJ.

In the next simulation, the performance of LMPC is analyzed and figure 4 shows the corresponding closed-loop dynamics. The optimized inputs given by the LMPC are strictly within the bounds and the reflux drum hold-up is also maintained within its limits. Due to the soft constraint on minimum product purity, the LMPC is able to handle trade off between production and energy consumption, resulting in higher values of PPI (0.3372) and EPI (21.46 kmol/GJ) compared to unconstrained LQR.

For the next simulation, the closed-loop dynamics of the VRBD column with the GLC scheme is considered and the corresponding responses are depicted in figure 5. The manipulations in the reflux rate are better handled due to the nonlinear control law, resulting in higher values of PPI (0.3572). As this controller does not penalize energy consumption, the EPI (17.14 kmol/GJ) is lower than LMPC.

In the last simulation run, multi-loop PI controllers are used during the production phase. Figure 6 depicts the corresponding closed-loop dynamics. The reflux rate given by PI controller in conventional control strategy increases almost linearly to maintain distillate purity at the desired value by consuming auxiliary reboiler duty. Interestingly, this scheme gives the best PPI of 0.3836 (which is even better than the nonlinear controller). However, this is accomplished by compromising benefits of energy integration and results in a small value of EPI (12.38 kmol/GJ).

Table 2 gives the comparison of performance for these control strategies. The LMPC has the highest EPI but a low value of PPI as it resulted in less amount of distillate. The PI controller, on the other hand, gave the highest PPI, but resulted in the least energy-efficient operation. The LMPC and GLC provided good trade-off between separation performance and energy efficiency.

5. CONCLUSION

In this paper, a comparison of model-based control strategies is presented for an energy-integrated batch distillation column. The operational objective of this system is to produce the maximum possible product at the desired purity with minimum energy consumption. We explored various model-based feedback control strategies and studied their closed-loop dynamics. Two key performance indicators were defined to compare separation yield and energy efficiency obtained during closed-loop response. All the model-based control strategies resulted in stable operation and satisfied the purity criteria. The LQR gave the most energy efficient operation (but with poor separation yield), whereas the multi-loop PI strategy resulted in the highest separation yield (with poor energy efficiency). The nonlinear GLC and linear MPC provided high values of both the performance indices. Motivated by this, to further improve these performance indices, we are currently working on the development of a nonlinear model predictive controller (NMPC) for this system.

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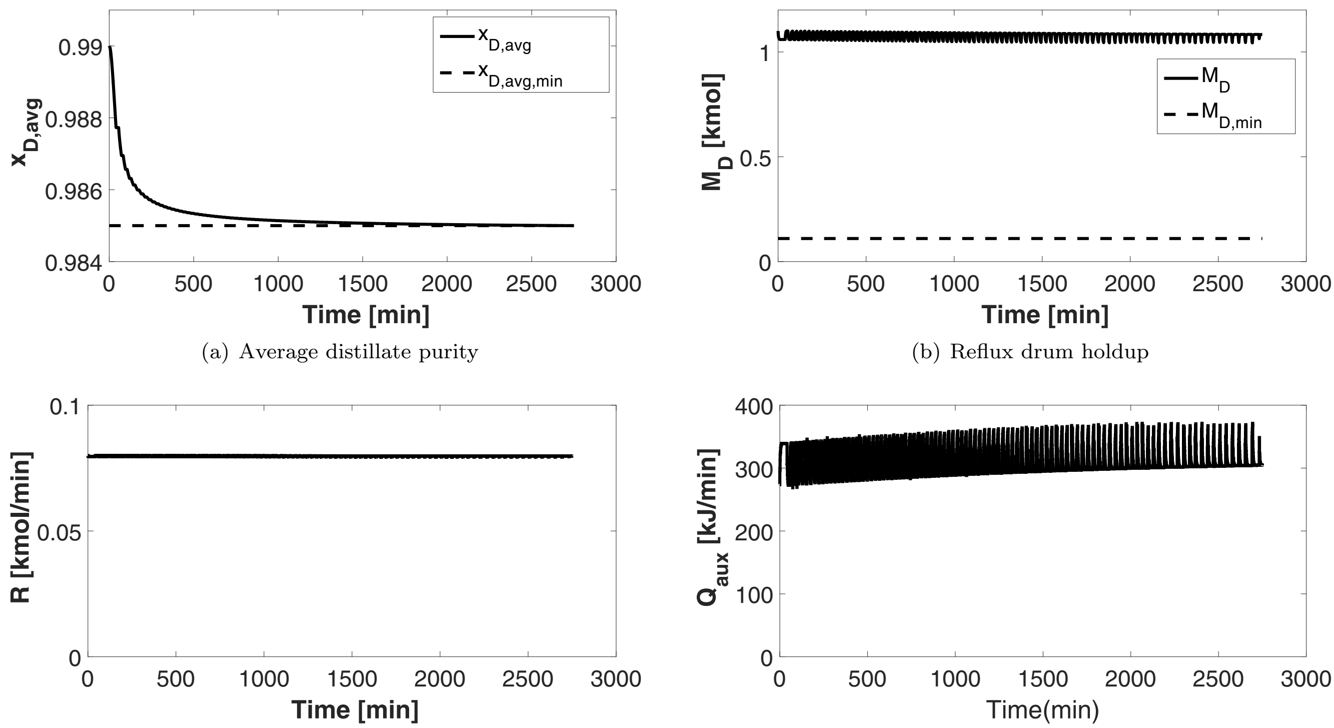


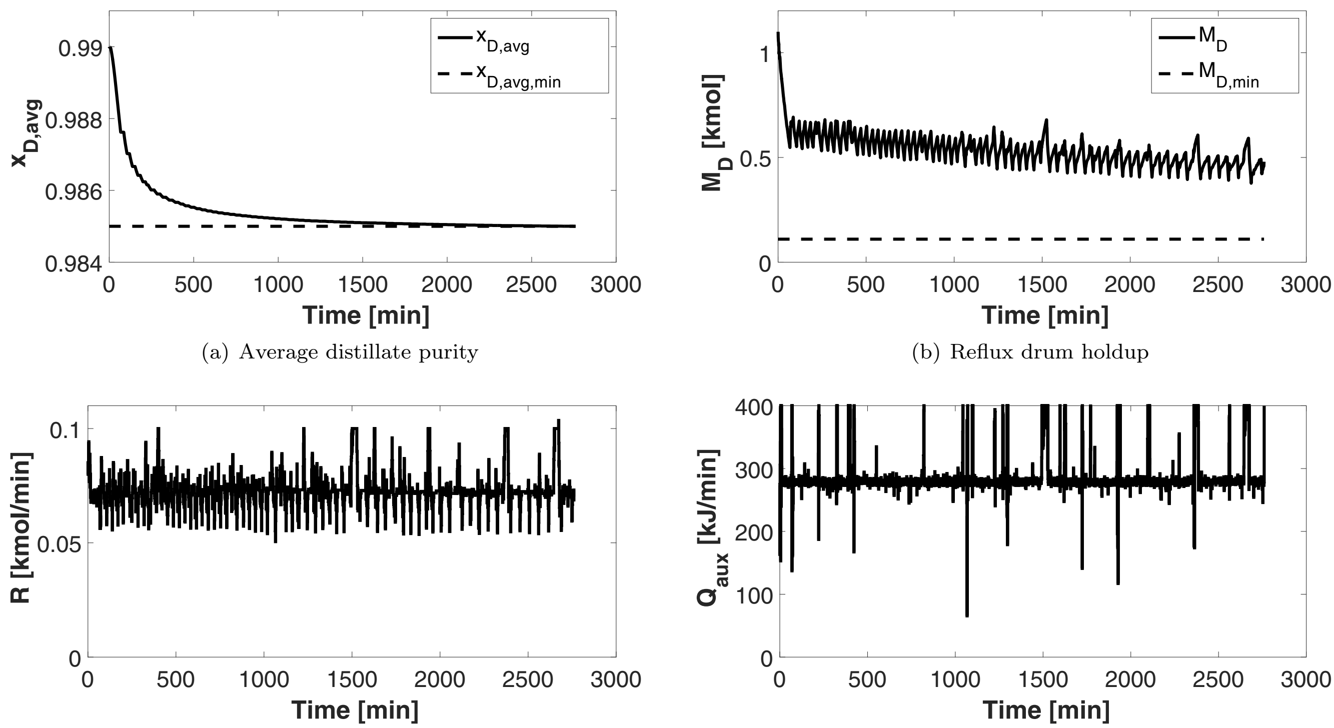
(a) Average distillate purity

(b) Reflux drum holdup

(c) Reflux rate

(d) Auxiliary reboiler duty

Fig. 3. Closed-loop response of the VRBD system with LQR in the production phase



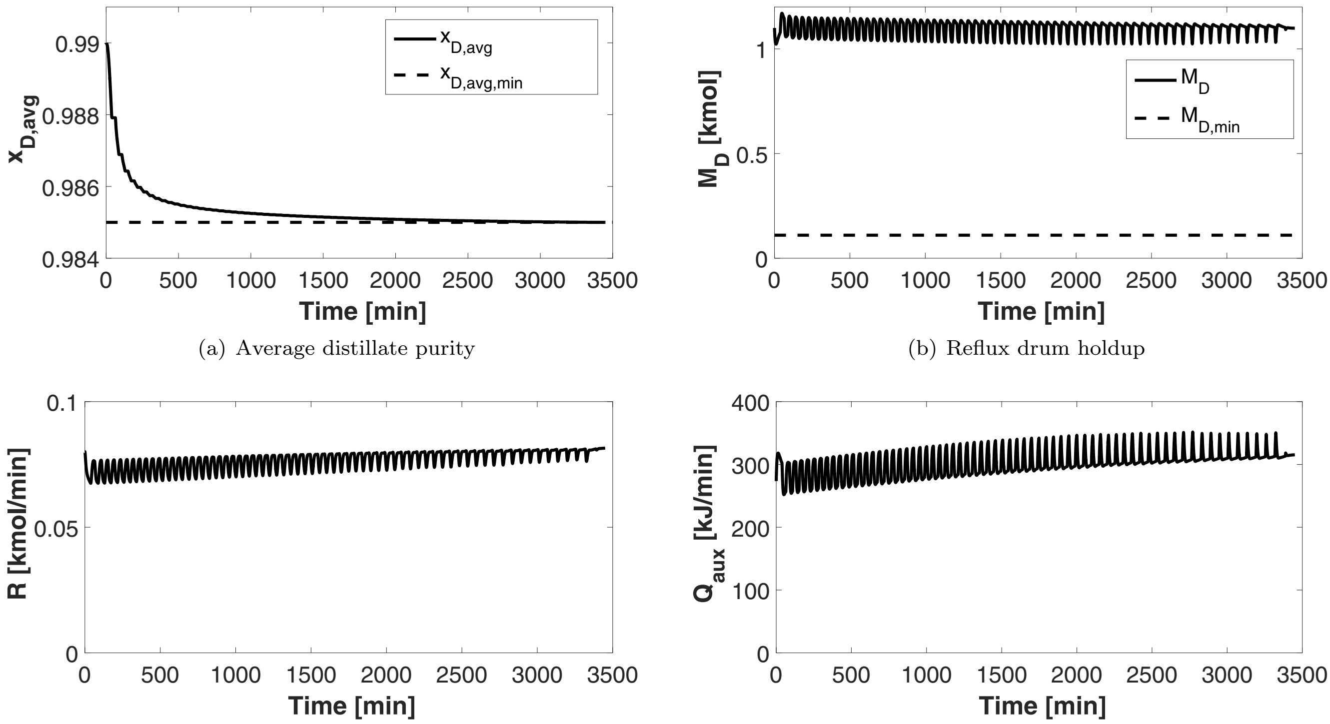
(a) Average distillate purity

(b) Reflux drum holdup

(c) Reflux rate

(d) Auxiliary reboiler duty

Fig. 4. Closed-loop response of the VRBD system with constrained LMPC in the production phase



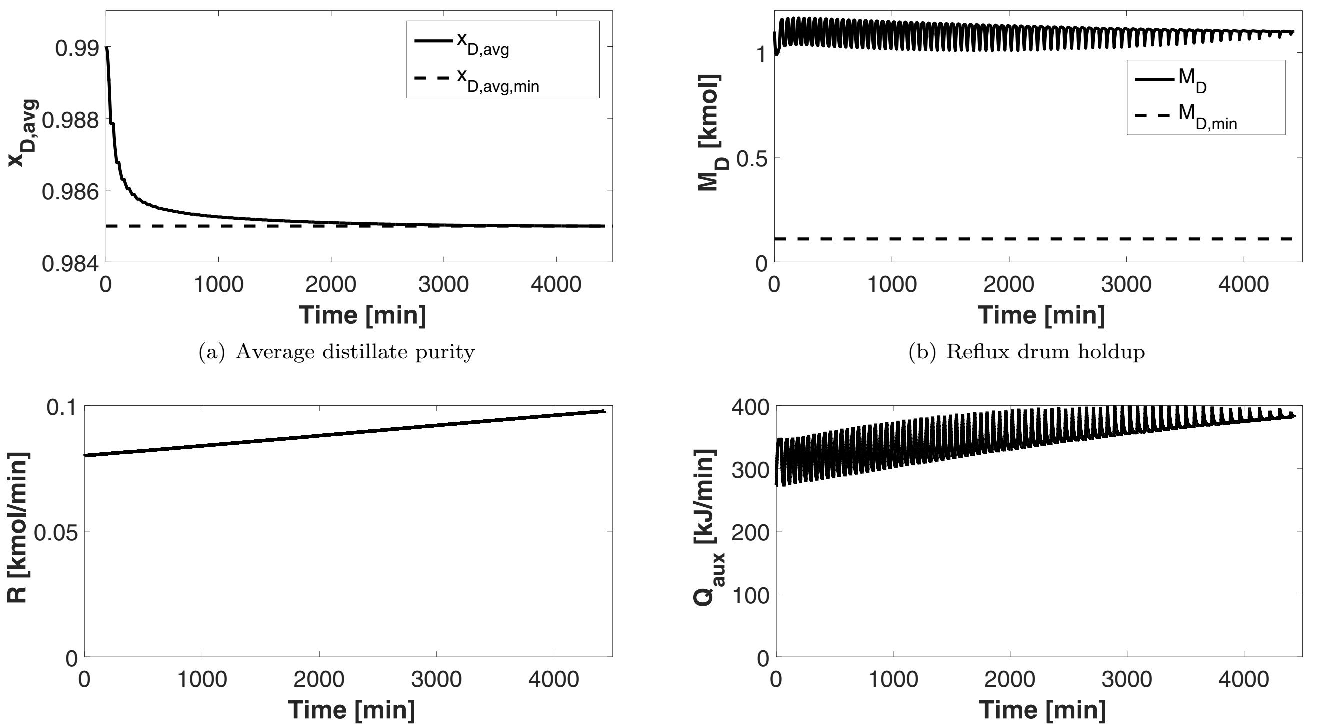
(a) Average distillate purity

(b) Reflux drum holdup

(c) Reflux rate

(d) Auxiliary reboiler duty

Fig. 5. Closed-loop response of the VRBD system with GLC in the production phase



(a) Average distillate purity

(b) Reflux drum holdup

(c) Reflux rate

(d) Auxiliary reboiler duty

Fig. 6. Closed-loop response of the VRBD system with multi-loop PI controllers in the production phase