



Article

Composition control and temperature inferential control of dividing wall column based on model predictive control and PI strategies☆

Jianxin Wang¹, Na Yu¹, Mengqi Chen¹, Lin Cong², Lanyi Sun^{1,*}¹ State Key Laboratory of Heavy Oil Processing, College of Chemical Engineering, China University of Petroleum (East China), Qingdao 266580, China² College of Information and Control Engineering, China University of Petroleum (East China), Qingdao 266580, China

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ABSTRACT

The dividing wall column (DWC) is considered as a major breakthrough in distillation technology and has good prospect of industrialization. Model predictive control (MPC) is an advanced control strategy that has acquired extensive applications in various industries. In this study, MPC is applied to the process for separating ethanol, *n*-propanol, and *n*-butanol ternary mixture in a fully thermally coupled DWC. Both composition control and temperature inferential control are considered. The multiobjective genetic algorithm function “gamultiobj” in Matlab is used for the weight tuning of MPC. Comparisons are made between the control performances of MPC and PI strategies. Simulation results show that although both MPC and PI schemes can stabilize the DWC in case of feed disturbances, MPC generally behaves better than the PI strategy for both composition control and temperature inferential control, resulting in a more stable and superior performance with lower values of integral of squared error (ISE).

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1. Introduction

Distillation is a widely used yet energy intensive separation technology in chemical industry. Given the high energy requirement, which accounts for over 50% of plant operating costs [1], a great number of researches have been done to improve the thermodynamic efficiency of distillation process. As is shown in Fig. 1, the separation for a ternary mixture has evolved from conventional distillation sequence to Petlyuk configuration and finally developed into the more integrated dividing wall column (DWC).

DWC is considered as a promising process intensification technology due to its potential to significantly reduce both energy requirement and equipment investment as well as an additional benefit of reducing required installation space [2–5]. Despite of all the remarkable advantages mentioned above, the highly interactive nature of DWC poses new challenges in terms of operability and controllability [3]. DWC has two more manipulated variables compared to the conventional distillation sequence: vapor and liquid split ratios, which need to be adjusted carefully during operation. What's more, the DWC integrates two columns into a single shell and eliminate the use of a reboiler and a condenser, causing the loss of degrees of freedom and strong interactions among variables. PI control is the most widely used multi-loop control strategy in

process industry. It calculates the control actions based on the linear combination of current and past deviations of the controlled variables. For the control of highly coupled nonlinear process like DWC, the PI strategy tends to deliver a relatively poor control quality due to the strong interactions between different control loops. Model predictive control (MPC) is an advanced control strategy. It obtains the control actions by solving an optimization problem based on a predictive model. Receding horizon optimization and feedback correction are also incorporated in the MPC algorithm to make up for the inaccuracy of the predictive model, which assures that MPC can be applied to the nonlinear and time varying process. Besides, it is a multi-input multi-output control scheme. Unlike the PI strategy, MPC takes into account the effect of all the manipulated variables on all the controlled variables simultaneously and therefore handles well the interactions between variables. All the features mentioned above make MPC a good candidate for the control of DWC.

There have been a large number of literatures addressing the control of DWC. Many of them are based on the multi-loop PI strategies. Mutalib and Smith [6] established two PI schemes for the control of DWC. Simulation result showed that stable control was achievable by both control schemes. Wang and Wong [7] explored the control of DWC based on PI schemes, demonstrating that there is a trade-off between energy efficiency and controllability. Ling and Luyben [8,9] studied the composition control and temperature control of the DWC for separating benzene/toluene/xylene (BTX) ternary mixture based on PI strategies. Buck *et al.* [10] applied decentralized PI schemes to a pilot DWC and demonstrated the effectiveness of the schemes. Kiss and Rewagad [11]

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* Corresponding author.

E-mail address: sunlanyi@upc.edu.cn (L. Sun).

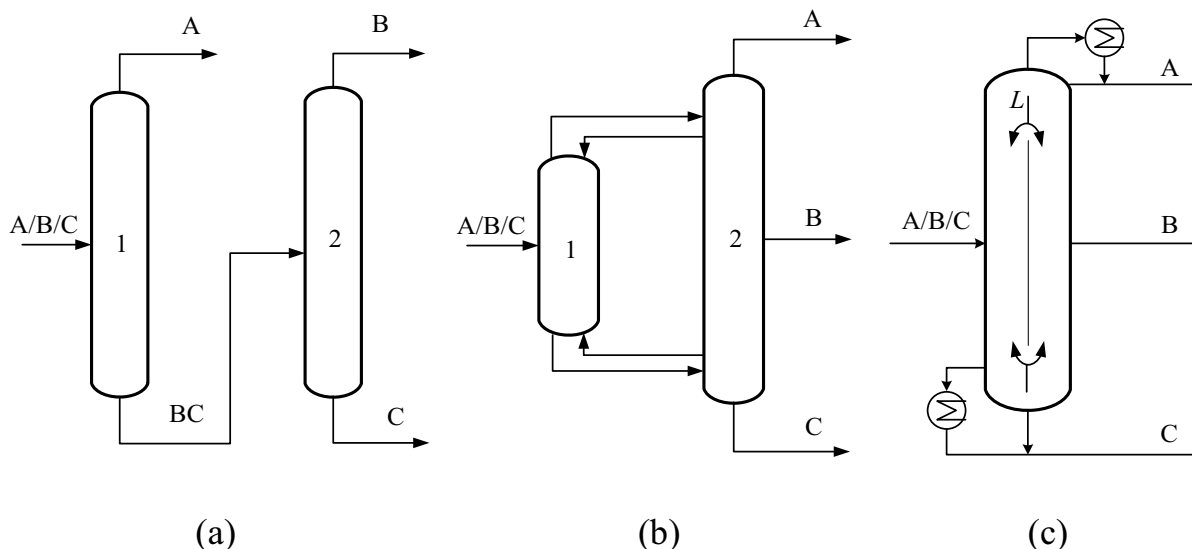


Fig. 1. Separation of a ternary mixture via (a) conventional distillation sequence, (b) Petlyuk configuration, (c) dividing wall column.

compared the performance of four PI control structures for the control of DWC. Xia *et al.* [12] confirmed the feasibility of using decentralized temperature and differential temperature control structures for the extractive DWC. Sun *et al.* [13] explored the control of extractive DWC for separating benzene/cyclohexane mixtures based on PI strategies. Qian *et al.* [14] applied PI schemes to the control of reactive DWC for selective hydrogenation and separation of C3 stream. Li *et al.* [15] explored the decentralized control of reactive DWC for hydrolysis of methyl acetate. Still there are some literatures investigating the control of DWC using MPC. Adrian *et al.* [16] investigated the model predictive control of the DWC for separating butanol/pentanol/hexanol system through experimental studies. Buck *et al.* [17] developed MPC for the operation of a pilot DWC for separating fatty alcohols *n*-hexanol, *n*-octanol, and *n*-decanol. Rewaged and Kiss [18] considered the separation of BTX in a DWC as a case study, exploring the control performances of conventional PI strategy and MPC scheme. Hernández and Chinea-Herranz [19] applied both PI strategy and MPC to a DWC. The separated ternary mixture consists of *n*-pentane, *n*-hexane, and *n*-heptane. Dohare *et al.* [20] chose the DWC for a BTX system as a case study and investigated the control behavior of MPC. Rodríguez *et al.* [21] applied MPC to the extractive DWC for bioethanol dehydration and the reactive DWC for the hydrolysis of methyl acetate to produce methanol and acetic acid. Another recent study on the application of MPC to reactive DWC is reported by Qian *et al.* [22]. MPC was proposed in their work for the control of the reactive DWC for the selective hydrogenation and separation of the C3 stream in ethylene production. Despite these studies investigate different DWC configurations and various systems, a similar conclusion can be reached that MPC generally performs better than the PI strategy. However, it should be pointed out that most of the above work focuses on composition control. Only a few papers deal with the temperature inferential control of DWC based on MPC. The absence of a comparison between the performances of MPC and PI strategies for the temperature inferential control of a pressure-driven DWC process justifies the work we did here. The aim of this work is to apply MPC to the control of the DWC for separating ethanol, *n*-propanol, and *n*-butanol ternary mixture and evaluate its control performance by comparison to its equivalent PI strategy. Both composition control and temperature inferential control are considered. PI control study is implemented in Aspen Dynamics. MPC control study is implemented by a joint simulation between Aspen Dynamics and Simulink in Matlab. The weights of controlled variables (w^y) and manipulated variables variations ($w^{\Delta u}$) for MPC are obtained by solving a multiobjective optimization problem through genetic algorithm (GA).

2. Process Description

The separation of ethanol (A), *n*-propanol (B), and *n*-butanol (C) is carried out in a DWC. As is shown in Fig. 2, a two-column model has been built as an equivalent flow sheet of the DWC. The RadFrac model in Aspen Plus is used for simulating the prefractionator (PC) and the main column (MC). Equilibrium stage model is adopted during simulation, which assumes the vapor and liquid phases leaving any stage are in thermodynamic equilibrium with each other. The assumption of no heat transfer across the dividing wall is also maintained. Pumps and valves have been added for a pressure-driven dynamic simulation, which is more in agreement with practical application than a flow-driven one. All valves are provided with sufficient pressure drop for effective dynamic controllability. Two fictitious compressors and pumps have been added to compensate the pressure drop.

The fresh feed comprising 20-mol% ethanol, 60-mol% *n*-propanol, and 20-mol% *n*-butanol is fed into the prefractionator at a flow rate of $100 \text{ kmol} \cdot \text{h}^{-1}$. Ethanol is distilled at the top of the main column, and *n*-propanol is withdrawn as side stream of the main column, while *n*-butanol is obtained as bottom product of the main column. Product purities are set to be 98 mol%. NRTL thermodynamic package is selected to account for the nonideal liquid phase behavior [7]. The initial values for all the parameters of the DWC are estimated from the conventional distillation sequence to obtain a converged Aspen Plus simulation. Sensitivity analysis is then implemented to find the parameters giving the minimum energy requirement. The flow rates of liquid (L_1) and vapor (V_2) are varied over a wide range. The reboiler duty which satisfies the specifications on the product purities is calculated accordingly. The simulation result shows that the range of L_1 from 30 to 50 and V_2 from 74 to 82 are in the feasible region for a converged simulation. Fig. 3 illustrates the effect of L_1 and V_2 on the reboiler duty. The minimum energy requirement occurs with the L_1 of $38.82 \text{ kmol} \cdot \text{h}^{-1}$ and V_2 of $78.91 \text{ kmol} \cdot \text{h}^{-1}$. Split ratio is defined as the ratio of the flow directed to the prefractionator to the flow directed to the main column. The resulting liquid split ratio (β_L) and vapor split ratio (β_V) are 0.385 and 1.177, respectively. The optimized parameters of the DWC are shown in Table 1.

3. Control of the Dividing Wall Column

In this section, dynamic control of the proposed DWC will be explored. Before converting the steady-state simulation to a pressure-driven dynamic simulation, it is necessary to specify the size of the

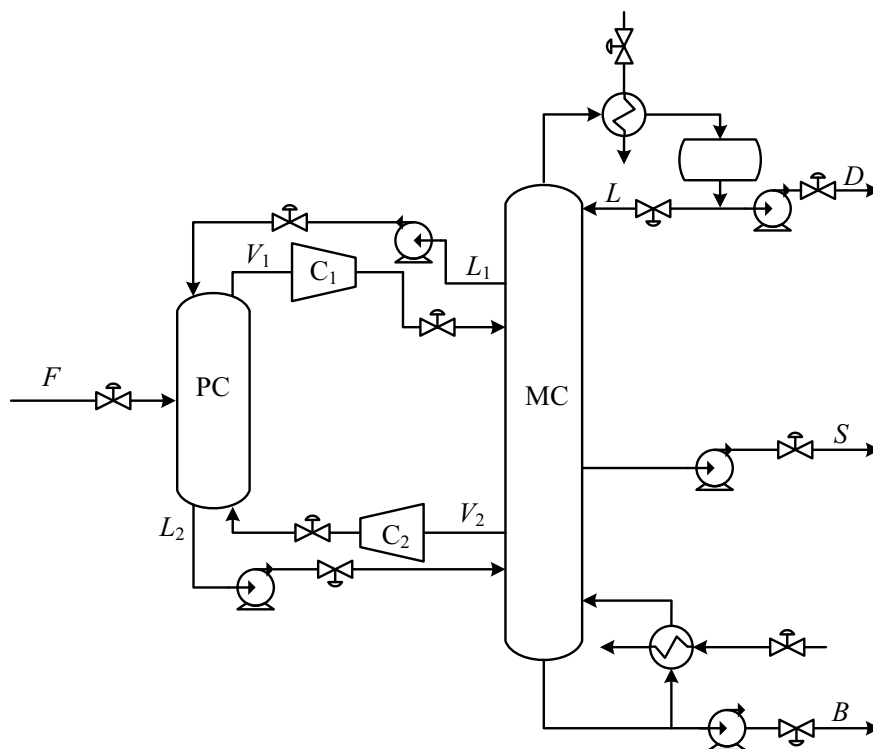


Fig. 2. Thermodynamically equivalent flow sheet of the DWC.

equipment. The tray sizing tool in Aspen Plus is used to calculate the column diameters. The reflux drum and the sump of each column are sized to provide 5-min holdup when half full. Most valves are specified to have pressure drops of 300 kPa with the valve half open at the design flow rate.

3.1. PI strategy

The conventional PI strategy comprises different control loops that can be divided into two levels. One is inventory control, which consists of liquid level, flow rate, and pressure control. It is used to guarantee the safety operation of the process since it is closely related to the material balance in the process. The other one is quality control, including composition and temperature control. It is used to maintain the product purity directly or indirectly.

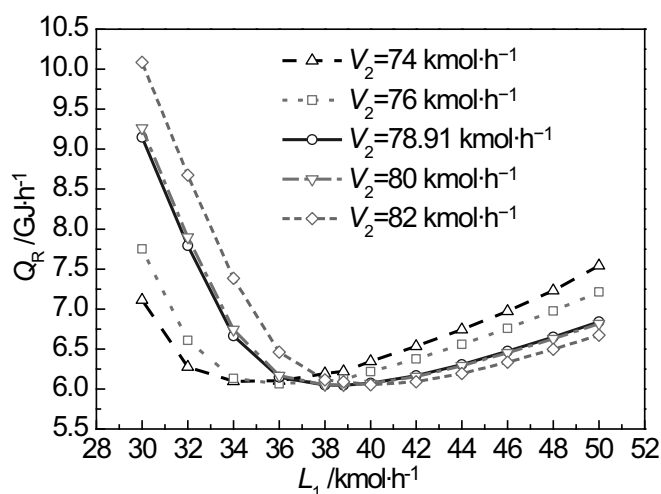


Fig. 3. Reboiler duty vs. liquid flow rate for different values of the vapor flow rate.

3.1.1. Composition control based on PI strategy

In this section, a composition control strategy with PI controllers is devised for the DWC. Following the report from Ling and Luyben [8], the liquid split ratio (β_L) is used as a manipulated variable to control the composition of the heavy component at the top of the prefractionator (y_C). Then, there are totally 9 manipulated variables and 9 controlled variables. The other controlled variables include the top stage pressure of the prefractionator (P_1) and main column (P_2), the liquid level in the reflux drum of the main column (L_{D2}), the sump level of the prefractionator (L_{B1}) and main column (L_{B2}), the mole fractions of ethanol in distillate (x_A), *n*-propanol in the side stream (x_B), and *n*-butanol in the bottom product (x_C). The rest of the manipulated variables include the condenser duty (Q_C) and reboiler duty (Q_R) of the main column, the reflux rate of the main column (L), the brake power of the compressor C_1 (m_1), the valve positions that affect the liquid flow rate L_2 (m_2), distillate flow rate D (m_3), side stream flow rate S (m_4) and bottom flow rate B (m_5). The key to an effective control

Table 1
Parameters for the DWC

Design parameter	Value
Prefractionator	
Number of trays	37
Feed tray	17
Top stage pressure/kPa	107.625
Main column	
Number of trays	60
Top feed/withdraw tray	9
Side stream product	28
Bottom feed/withdraw tray	47
Top stage pressure/kPa	101.325
Reflux ratio	7.52
Liquid to prefractionator, $L_1/\text{kmol}\cdot\text{h}^{-1}$	38.82
Vapor to prefractionator, $V_2/\text{kmol}\cdot\text{h}^{-1}$	78.91
Reboiler duty $\times 10^{-6}/\text{kJ}\cdot\text{h}^{-1}$	6.058
Condenser duty $\times 10^{-6}/\text{kJ}\cdot\text{h}^{-1}$	6.741

composition of *n*-butanol at the top of the prefractionator (y_C) is controlled by manipulating the liquid split ratio (β_L).

Since the composition measurements often suffer from large delays in an industrial environment, a 3-min dead time is inserted into the four composition control loops to improve the realism of the simulation [13]. Relay-feedback test is carried out to determine the ultimate gain and period. Tyreus-Luyben tuning rules are used to calculate proportional gain and integral time. Tuning results for the four composition controllers are shown in Table 3.

Table 3
Tuning results for composition controllers

	Controlled variable	Manipulated variable	Proportional gain K_C	Integral time τ_I/min
CC1	x_A	L/F	3.98	63.4
CC2	x_B	m_4	14.04	23.8
CC3	x_C	Q_R/F	2.39	60.7
CC4	y_C	β_L	0.18	26.4

3.1.2. Temperature inferential control based on PI strategy

In this section, temperature inferential control is considered for wider industrial applications. A classic three-point temperature control structure is built. The sensitivity criterion is used to select temperature sensitive trays. It is performed as follows: the L , Q_R and S are manipulated for the purpose of control. A small change (0.1%) is made in L with Q_R and S being fixed. Aspen Plus simulation is run, giving a new temperature profile. The temperature change of tray i (ΔT_i) is obtained by subtracting the initial temperature from the new one. Dividing (ΔT_i) by the change of L gives the steady-state gain on tray i . Repeating this procedure for the other manipulated variables gives other two gains. The steady-state gains are plotted against tray number in Fig. 5. The

trays with relatively large gains reflect the appropriate locations to be temperature-controlled. The controlled temperatures are selected at stages 8 (T_8), 36 (T_{36}), and 55 (T_{55}). As shown in Fig. 5, both T_8 and T_{55} are sensitive to L and Q_R , but a change in the reflux rate L takes a longer time to affect the temperature on the 55th tray because of liquid hydraulic lags. The principle of proximity is therefore followed to determine the variables pairing. Fig. 6 shows the proposed temperature inferential control structure.

T_8 in the main column is controlled by manipulating the ratio of the reflux rate to the feed flow rate (L/F). T_{36} and T_{55} in the main column are maintained by manipulating m_4 and the ratio of the reboiler duty to the feed flow rate (Q_R/F), respectively. Comparing with composition control, temperature control brings in shorter drag time. One minute of dead time is inserted into all temperature control loops to fit the practical operation [12]. The settings for the inventory control loops including pressure, liquid level and feed flow rate control are the same as those of the composition control structure mentioned earlier. Table 4 lists the tuned parameters of the temperature controllers.

3.2. Theory of model predictive control

Model predictive control is a model-based optimization algorithm. It optimizes over p future sampling periods and calculates m future control actions at each sampling instant. The estimated state variables are used as initial conditions at each sampling instant. The optimal control sequence that minimizes the objective function and fulfills the constraints is obtained at each sampling instant by solving a finite horizon open-loop optimal control problem. Only the first control action in the sequence is applied to the plant. The prediction horizon p and control horizon m then proceed forward by one sampling interval. The model is updated based on the new measurements and current states at each sampling instant, and then the calculations are repeated, yielding a new control sequence.

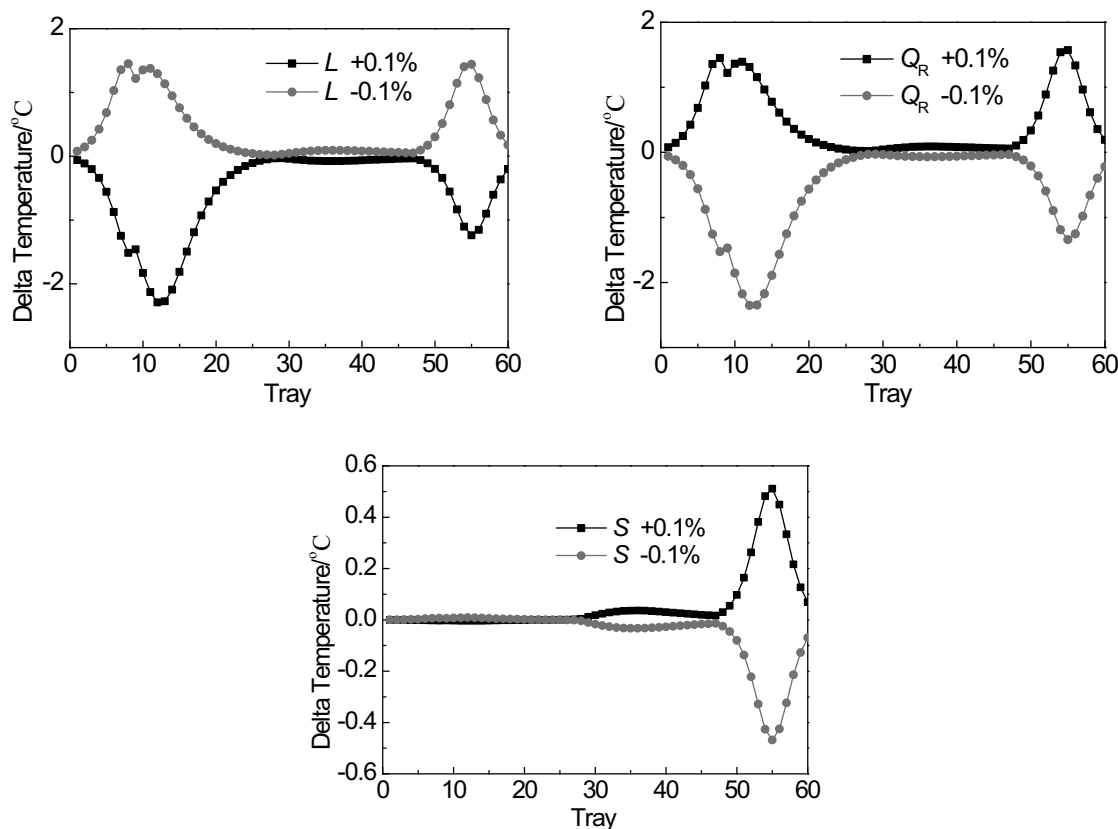


Fig. 5. Open-loop sensitivity analysis between manipulated variables and tray temperature changes.

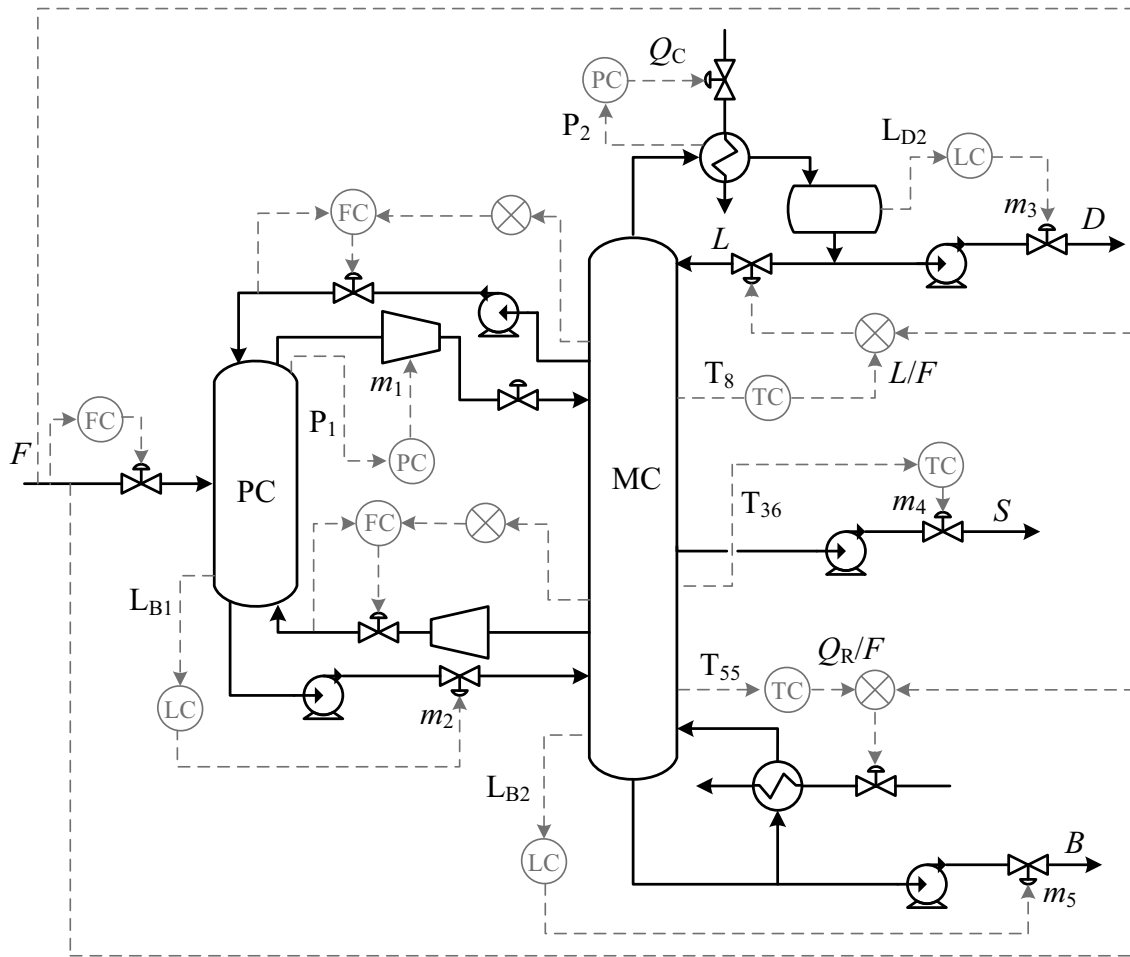


Fig. 6. Temperature inferential control structure based on PI loops.

In this study, a state space model, which is compact and convenient for representing multivariable systems, is used to describe the real plant model:

$$\mathbf{x}(k+1) = \mathbf{A}\mathbf{x}(k) + \mathbf{B}_u\mathbf{u}(k) + \mathbf{B}_v\mathbf{v}(k) + \mathbf{B}_d\mathbf{d}(k) \quad (1)$$

$$\mathbf{y}_m(k) = \mathbf{C}_m\mathbf{x}(k) + \mathbf{D}_{vm}\mathbf{v}(k) + \mathbf{D}_{dm}\mathbf{d}(k) \quad (2)$$

$$\mathbf{y}_u(k) = \mathbf{C}_u\mathbf{x}(k) + \mathbf{D}_{vu}\mathbf{v}(k) + \mathbf{D}_{du}\mathbf{d}(k) \quad (3)$$

where $\mathbf{x}(k)$ represents the vector of state variables; $\mathbf{u}(k)$ is the vector of manipulated variables; $\mathbf{v}(k)$ denotes the vector of measured disturbances; $\mathbf{d}(k)$ is the vector of unmeasured disturbances; $\mathbf{y}_m(k)$ refers to the vector of measured outputs; $\mathbf{y}_u(k)$ indicates the vector of unmeasured outputs. The model matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ are obtained by linearization of the rigorous, nonlinear dynamic model built in Aspen Dynamics through the Control Design Interface (CDI) tool. For the process studied here, the resulting linear model has over 500 state variables, representing the total enthalpy at each tray, molar quantity of each component at each tray, and variables of other blocks such as

valves. To avoid the difficulty of implementing the calculation with such a large number of variables, model reduction is carried out to reduce the number of state variables, which speeds up the calculations with negligible effect on prediction accuracy.

The optimization problem to be solved at each sampling instant is defined as follows:

$$\Delta u(k|k), \dots, \Delta u(m-1+k|k), \varepsilon \left\{ \begin{aligned} & \sum_{j=1}^{n_y} \left| w_{i+1,j}^y (y_j(k+i+1|k) - r_j(k+i+1)) \right|^2 \\ & + \sum_{j=1}^{n_u} \left| w_{i,j}^{du} \Delta u_j(k+i|k) \right|^2 \\ & + \sum_{j=1}^{n_u} \left| w_{i,j}^u (u_j(k+i|k) - u_{jt \text{ target}}(k+i)) \right|^2 \end{aligned} \right\} + \rho_e \varepsilon^2 \quad (4)$$

In the above equation, m is the control horizon over which the manipulated variables are allowed to change. p is the prediction horizon over which the optimization is performed. The subscript j denotes the j component of a vector. $(k+i|k)$ denotes the value predicted for time $k+i$ based on the information available at time k . $r(k)$ is the current sample of the output reference.

In this work, the sampling interval is set to be small enough to reproduce the total dynamic. The prediction horizon p and control horizon m , which are expressed in the form of the number of sampling intervals, are determined to keep the process stable with less oscillation.

The weights w^u , w^y , and w^{du} determine the relative penalizations for the deviations of manipulated variables, controlled variables from their nominal values, and manipulated variables variations, respectively. In this work, the number of manipulated variables is equal to that of

Table 4
Tuning results for temperature controllers

	Controlled variable	Manipulated variable	Proportional gain K_c	Integral time τ_I/min
TC1	T_8	L/F	1.83	13.2
TC2	T_{36}	m_4	36.91	10.6
TC3	T_{55}	Q_R/F	2.87	9.24

controlled variables. All the manipulated variables are expected to deviate from their nominal value in order to drive all the controlled variables to the set point values when disturbances occur. Therefore, w^u are set to 0. w^y and $w^{\Delta u}$ are determined by a tradeoff between two opposite aspects. In general, large values of w^y and small values of $w^{\Delta u}$ allow the controller to react with aggressive control actions, and shorter settling times can be achieved, but the tendencies for oscillation and overshoots increase. Small values of w^y and large values of $w^{\Delta u}$ will force the controller to behave more conservatively, which may reduce oscillation and overshoots but lead to longer settling times. The tuning of the weights can be defined as a multiobjective optimization problem. A discrete set of the Pareto optimum solution can be obtained by solving the problem. The weights corresponding to a control performance that is not too aggressive and additionally not too defensive can be chosen as the final solution.

In this work, the values of w^y and $w^{\Delta u}$ are tuned by solving the multiobjective optimization problem through “gamultiobj” function in Matlab. “gamultiobj” uses a controlled elitist genetic algorithm which is a variant of NSGA-II. The sum of squared errors of controlled variables and the sum of squared values of manipulated variables variations are defined as two objective functions:

$$\min \text{obj } 1 = \sum [y(k) - r(k)]^2 \quad (5)$$

$$\min \text{obj } 2 = \sum [\Delta u(k)]^2 \quad (6)$$

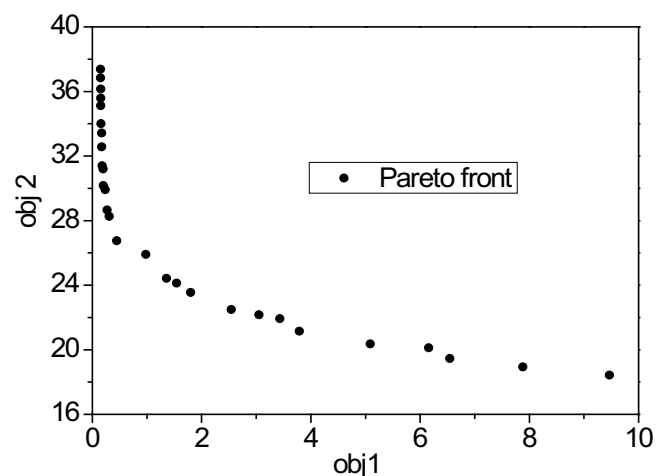


Fig. 8. Pareto optimum solution set for composition control.

For the convenience of weight tuning, all the input and output variables have been converted to a uniform dimensionless scale (0–100) with a nominal value of 50. A base value of 0 is selected for the conversion of all the variables. The model matrices B and C have also been scaled in accordance with the scaled variables.

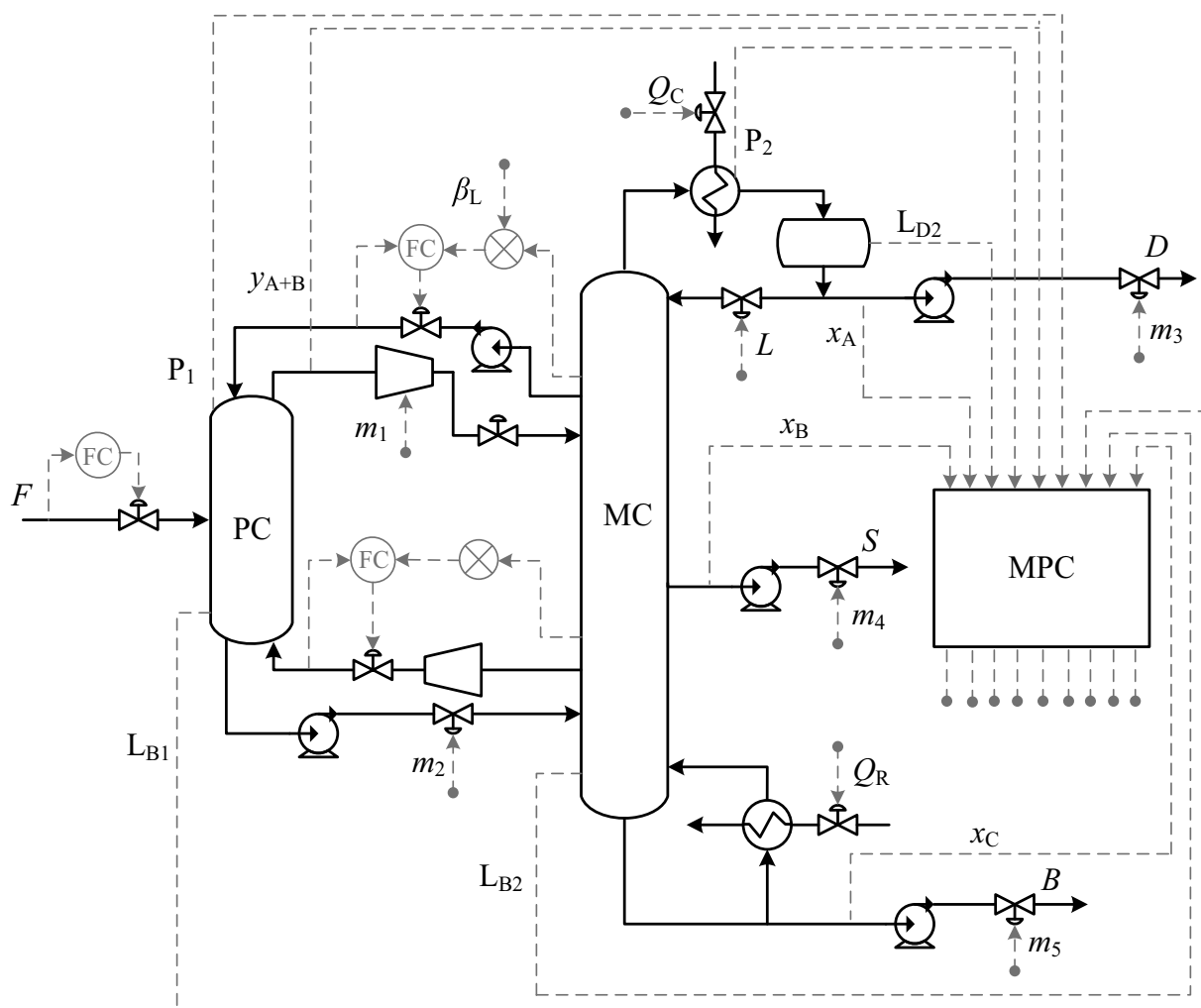


Fig. 7. Composition control structure for MPC.

Table 5
Summary of controller parameters for composition control

Controller parameters									
Sampling interval Δk			Prediction horizon p			Control horizon m			
0.01 h			4			50			
Weights									
U	Q_C	m_1	Q_R	L	m_4	β_L	m_3	m_5	m_2
w^u	0	0	0	0	0	0	0	0	0
$w^{\Delta u}$	6.0842	6.1826	8.0396	10.7349	4.1884	13.0206	7.5689	1.6507	10.4266
Y	P_2	P_1	x_C	x_A	x_B	$y_A + B$	L_{D2}	L_{B2}	L_{B1}
w^y	12.0811	13.3360	11.6598	15.3941	13.4331	14.3346	12.3069	14.9587	4.3509
Constraints									
Y	P_2	P_1	x_C	x_A	x_B	$y_A + B$	L_{D2}	L_{B2}	L_{B1}
	—	—	—	—	—	—	25–75	25–75	25–75
U	Q_C	m_1	Q_R	L	m_4	β_L	m_3	m_5	m_2
	0–100	0–100	0–100	0–100	0–100	0–100	0–100	0–100	0–100

3.2.1. Composition control based on model predictive control

The composition control structure for MPC is shown in Fig. 7. It should be pointed out that the content of *n*-butanol at the top of the prefractionator (y_C) is at a very low level with a steady state value of 0.0066 (mole fraction), and it is sensitive to the disturbances in the process. Relatively large deviation from the steady state value will occur in case of 10% feed disturbances. However, the accuracy of the linear model is usually acceptable around the point where the linearization is carried out. For the case away from the steady-state operating point, the linear model can't approach the complicated nonlinear relationship

sufficiently. Since MPC calculates the control sequence based on the linear model and the feedback of the controlled variables, the large variations of the controlled variables combined with the inaccurate linear model may result in an inappropriate control sequence, causing the instability of the process. A solution to the problem is to control the summation of the content of ethanol and *n*-propanol at the top of the prefractionator ($y_A + B$). Fig. 8 shows the resultant Pareto optimum solution set for composition control. The value of obj 1 reflects the control performance of MPC. The value of obj 2 is an indicator of the change rates of manipulated variables. Considering the relative importance of

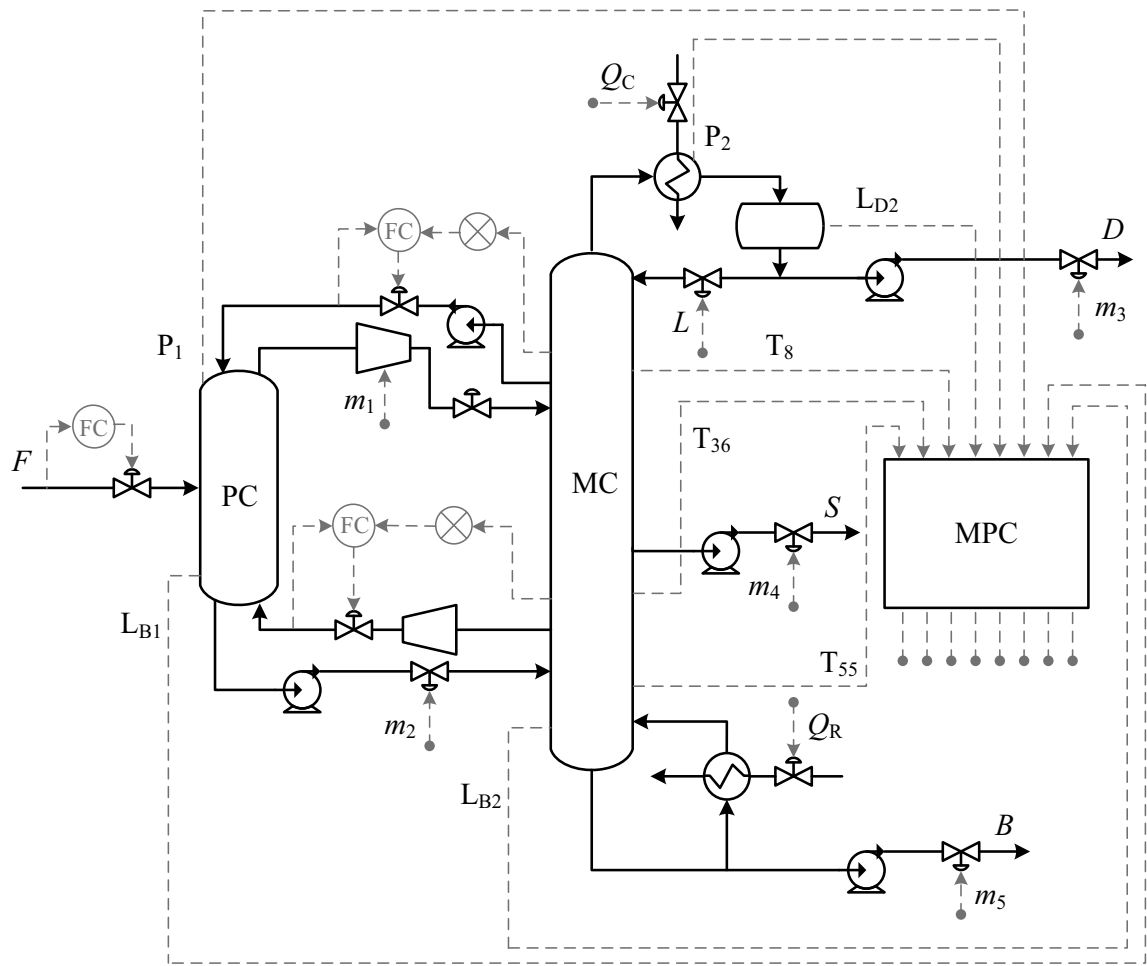


Fig. 9. Temperature inferential control structure for MPC.

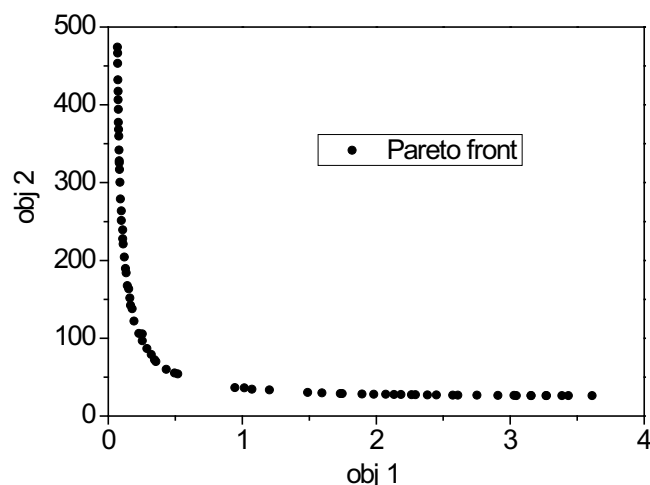


Fig. 10. Pareto optimum solution set for temperature inferential control.

Table 6

Summary of controller parameters for temperature inferential control

Controller parameters									
Sampling interval Δk			Prediction horizon p				Control horizon m		
0.01 h			4				50		
Weights									
U	Q_C	m_1	Q_R	L	m_4	m_3	m_5	m_2	
w^u	0	0	0	0	0	0	0	0	
$w^{\Delta u}$	0.2000	0.3051	0.2027	0.2070	0.2147	0.2369	0.1117	0.3609	
Y	P_2	P_1	T_{55}	T_8	T_{36}	L_{D2}	L_{B2}	L_{B1}	
w^y	3.2656	3.1064	4.5701	4.2679	1.7452	4.6120	2.7938	4.2083	
Constraints									
Y	P_2	P_1	T_{55}	T_8	T_{36}	L_{D2}	L_{B2}	L_{B1}	
	–	–	–	–	–	25–75	25–75	25–75	
U	Q_C	m_1	Q_R	L	m_4	m_3	m_5	m_2	
	0–100	0–100	0–100	0–100	0–100	0–100	0–100	0–100	

the two objective functions, more emphasis is put on the minimization of obj1 to improve the control performance of MPC. The point corresponding to an obj 1 value of 0.28 and an obj 2 value of 31.24 is chosen as the final solution. The tuning parameters of MPC are listed in Table 5.

3.2.2. Temperature inferential control based on model predictive control

The temperature inferential control structure for MPC and the resulting Pareto optimum solution set are shown in Figs. 9 and 10, respectively. The point corresponding to an obj 1 value of 0.0732 and an obj 2 value of 427.47 is chosen as the final solution. The tuning parameters of MPC are listed in Table 6.

4. Results and Discussions

Dynamic simulations are conducted to test the control performance of the proposed MPC scheme and compare it with that of PI scheme; $\pm 10\%$ step changes in feed flow rate and feed composition are introduced as persistent disturbances at 0.5 h.

4.1. Composition control

Figs. 11 to 14 show dynamic responses of the MPC vs. those of PI strategy for composition control to disturbances in feed flow rate and feed composition. It can be seen that both schemes can achieve the goal to steer the system to the given set points, but MPC shows better performance in maintaining product purities, featured with reduced overshoots, less oscillation and shorter settling times. The responses of the manipulated variables to $\pm 10\%$ step changes in feed flow rate are shown in Fig. 15. As can be seen, MPC reacts as quickly as the PI strategy to the feed flow rate disturbances, and the manipulated variables move more smoothly and reach new steady states in a shorter time. The following reasons may account for the improved control quality of MPC: (1) MPC takes into account simultaneously the effects of all manipulated variables to all controlled variables; thus, a coordination between manipulated variables is possible, which is helpful to reduce the oscillation. (2) The measured disturbances and the use of the prediction

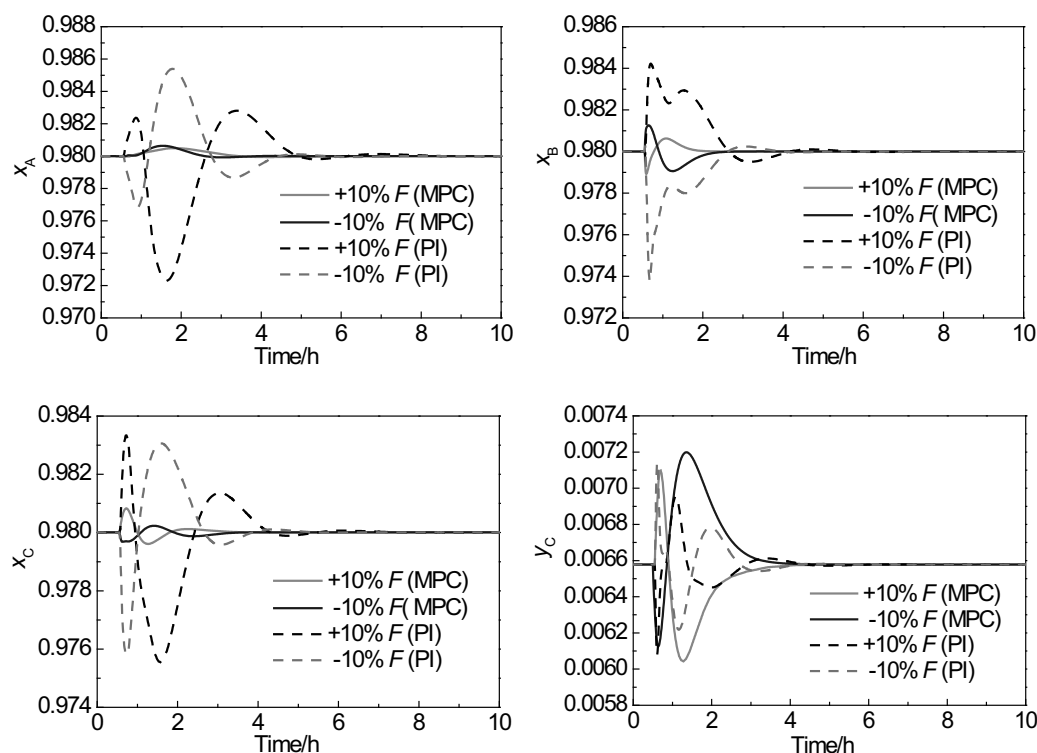


Fig. 11. MPC vs. PI for composition control: dynamic responses to $\pm 10\%$ feed flow rate disturbances.

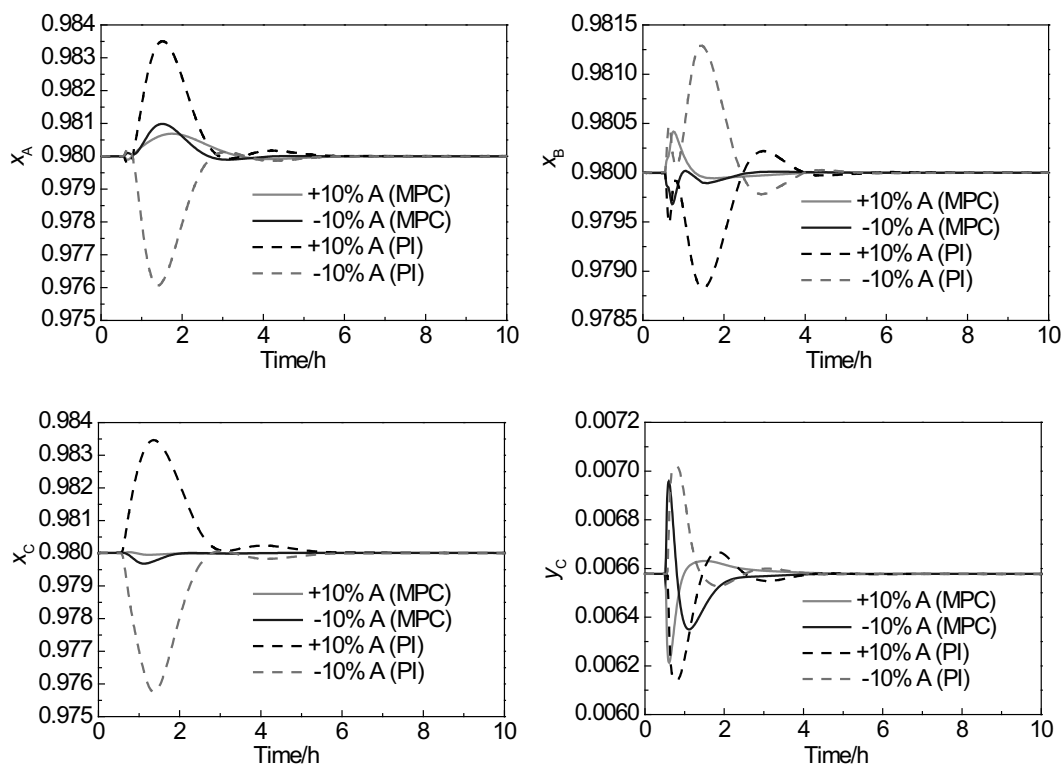


Fig. 12. MPC vs. PI for composition control: dynamic responses to $\pm 10\%$ feed composition of ethanol disturbances.

model assure a feed-forward control and optimized control actions. A more stable and superior performance can therefore be obtained.

For the feed flow rate disturbances, the liquid split ratio ends up at a new steady-state value with a negligible difference from the initial

value. The small deviation is due to the change of the pressure in the DWC. Since the throughput changes while the size of the column remains unchanged, the pressure profile in the column will also change since the pressure drop at each tray varies with the vapor and liquid

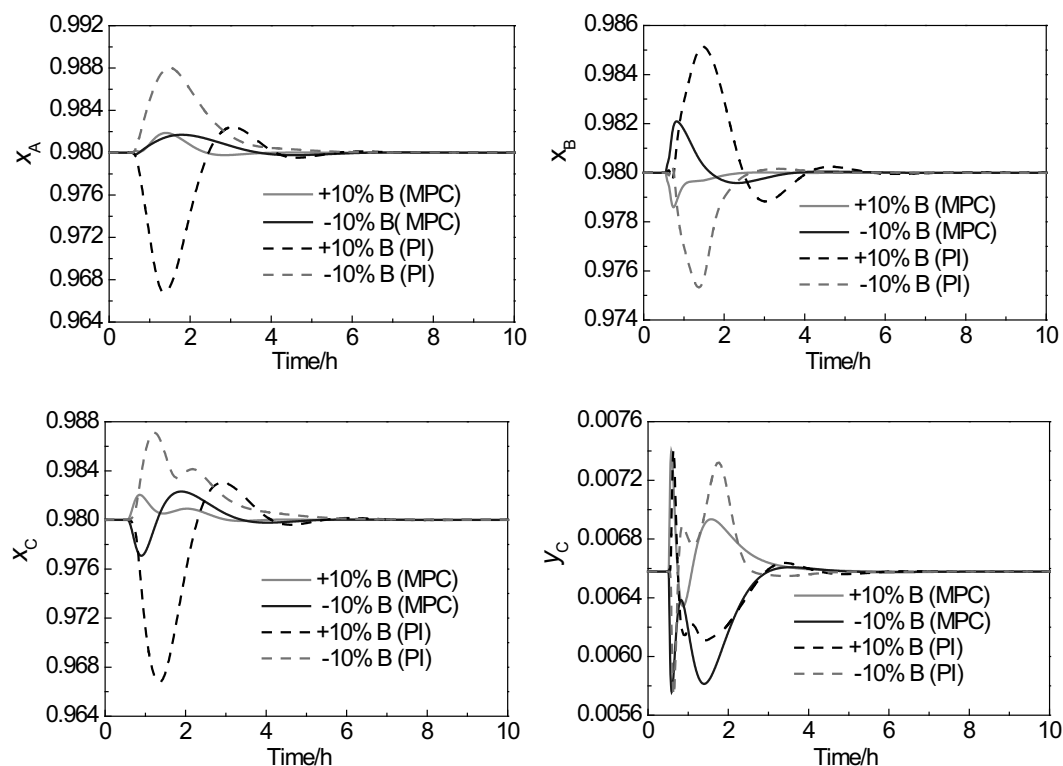


Fig. 13. MPC vs. PI for composition control: dynamic responses to $\pm 10\%$ feed composition of *n*-propanol disturbances.

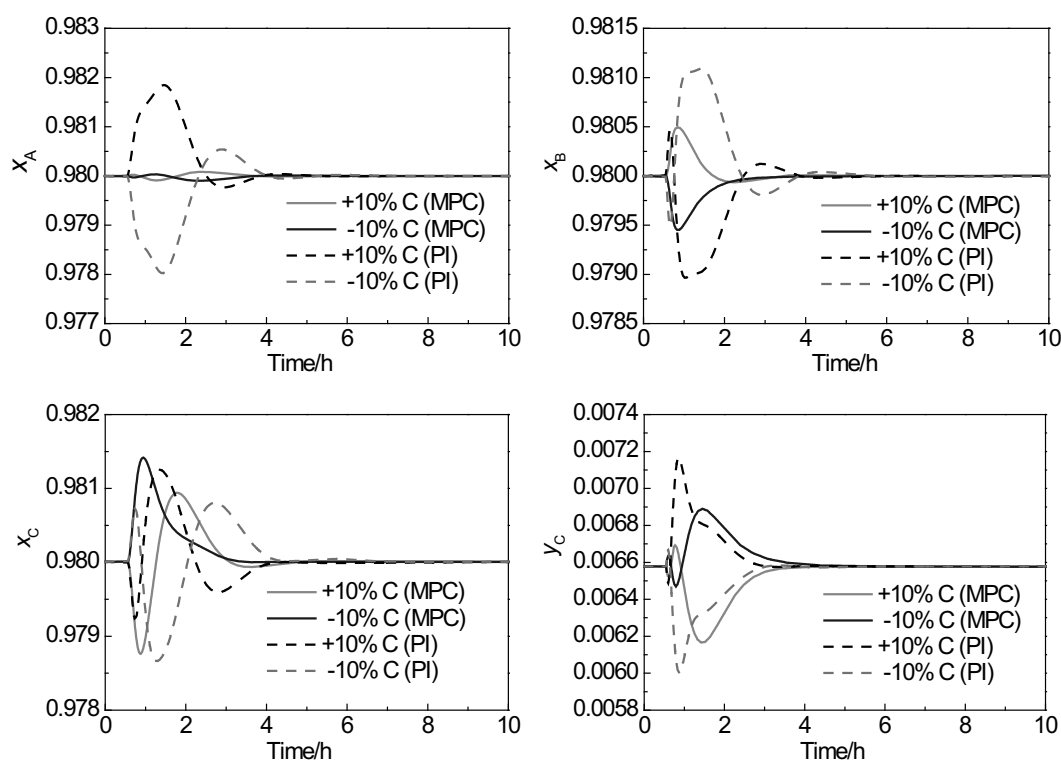


Fig. 14. MPC vs. PI for composition control: dynamic responses to $\pm 10\%$ feed composition of *n*-butanol disturbances.

rates in the column. The change of the pressure profile will inevitably lead to the changes of temperature and composition profile in the column. The deviations of the manipulated variables are therefore

required to steer the process to the new steady state. The manipulated variables L , S , and Q_R all reach new values that are 10% higher or lower than the original.

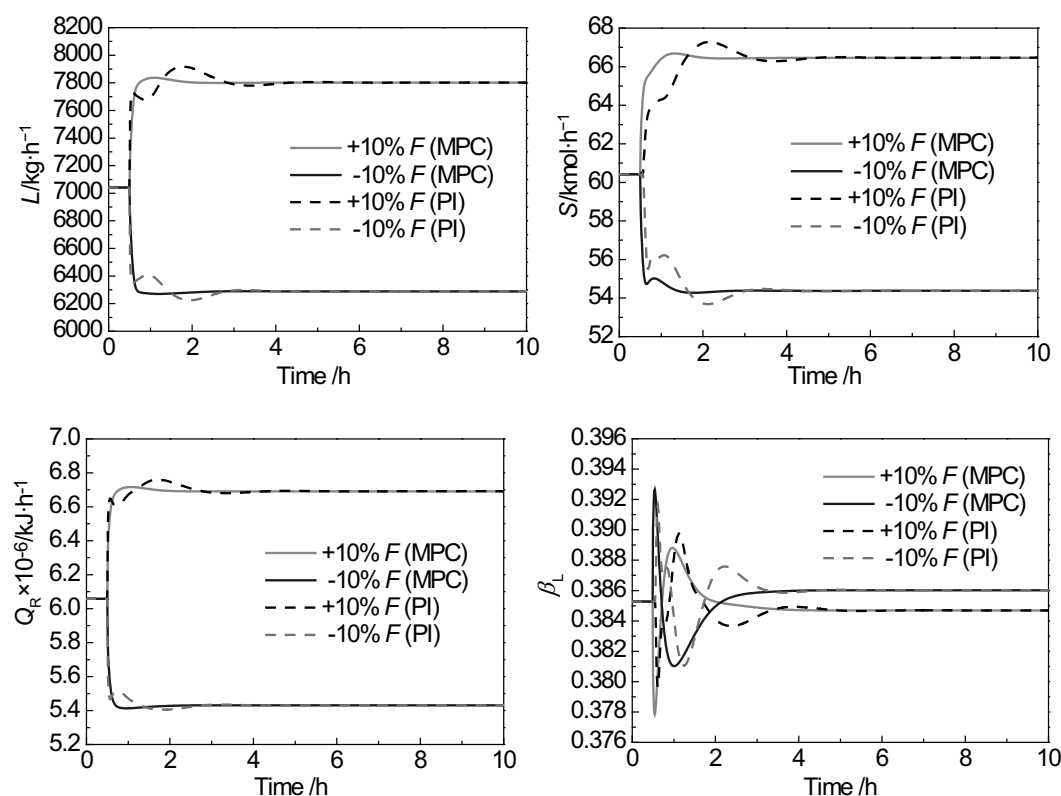


Fig. 15. MPC vs. PI for composition control: dynamic responses of manipulated variables when $\pm 10\%$ feed flow rate disturbances occur.

Table 7

Comparison of the performance of MPC vs. PI control for composition control in terms of the ISE

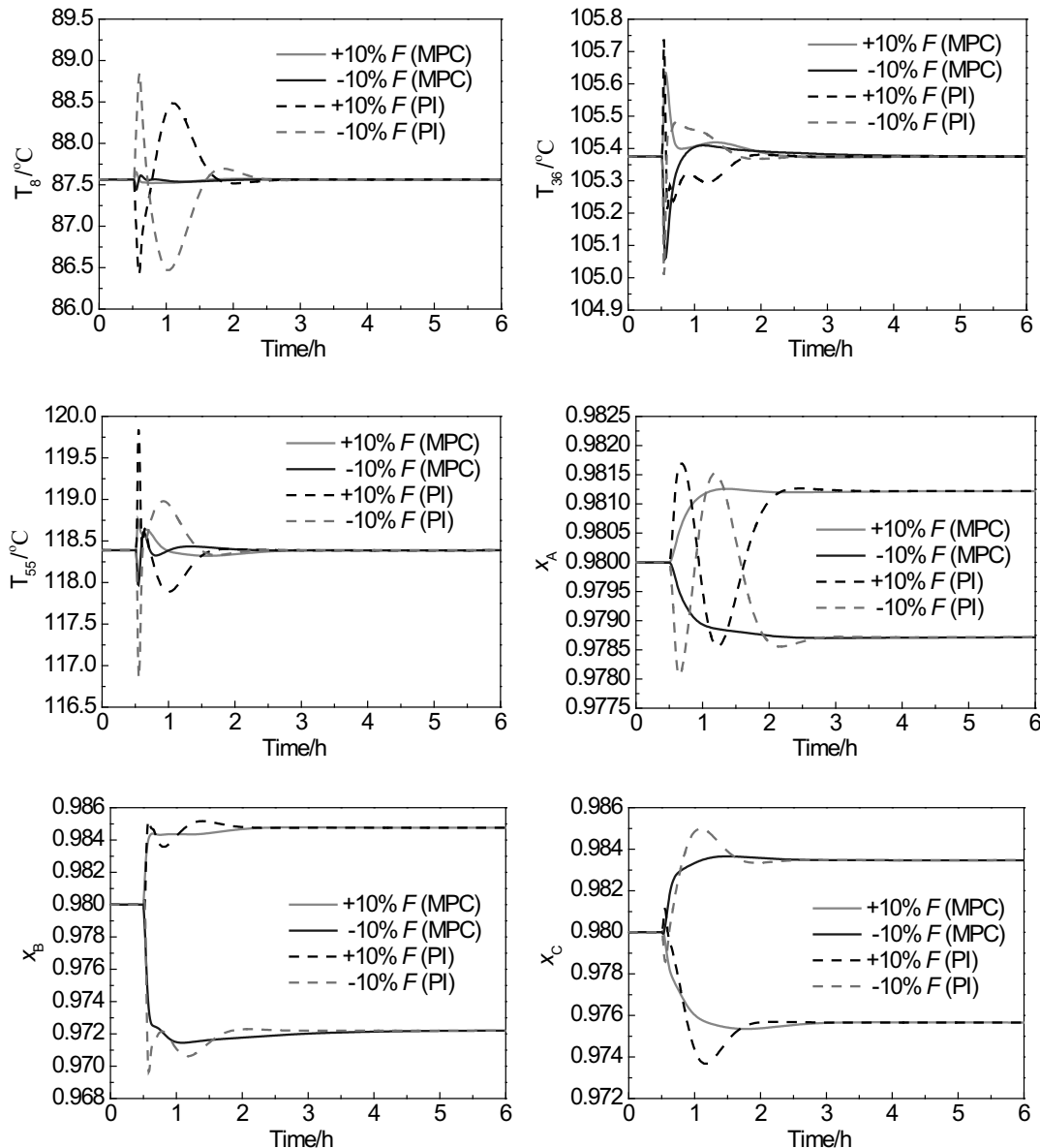
Disturbance	x_{A_PI}	x_{A_MPC}	x_{B_PI}	x_{B_MPC}	x_{C_PI}	x_{C_MPC}	y_{C_PI}	y_{C_MPC}
+10% F	1.40×10^{-5}	2.81×10^{-7}	1.28×10^{-5}	2.63×10^{-7}	1.65×10^{-5}	2.10×10^{-7}	6.19×10^{-8}	2.17×10^{-7}
−10% F	1.05×10^{-5}	3.08×10^{-7}	1.04×10^{-5}	7.65×10^{-7}	1.10×10^{-5}	6.52×10^{-8}	8.37×10^{-8}	3.40×10^{-7}
+10% A	1.19×10^{-5}	5.60×10^{-7}	1.18×10^{-6}	4.57×10^{-8}	1.48×10^{-5}	2.04×10^{-9}	7.35×10^{-8}	2.49×10^{-8}
−10% A	1.29×10^{-5}	7.55×10^{-7}	1.13×10^{-6}	2.27×10^{-8}	1.81×10^{-5}	5.46×10^{-8}	8.47×10^{-8}	4.65×10^{-8}
+10% B	1.35×10^{-4}	2.39×10^{-6}	2.23×10^{-5}	4.95×10^{-7}	1.31×10^{-4}	2.14×10^{-6}	3.02×10^{-7}	1.76×10^{-7}
−10% B	6.88×10^{-5}	3.85×10^{-6}	1.32×10^{-5}	1.97×10^{-6}	4.44×10^{-5}	7.59×10^{-6}	3.74×10^{-7}	5.44×10^{-7}
+10% C	3.23×10^{-6}	1.00×10^{-8}	9.89×10^{-7}	1.11×10^{-7}	1.25×10^{-6}	1.13×10^{-6}	1.49×10^{-7}	1.35×10^{-7}
−10% C	3.53×10^{-6}	9.37×10^{-9}	1.16×10^{-6}	1.54×10^{-7}	1.72×10^{-6}	1.12×10^{-6}	1.57×10^{-7}	8.26×10^{-8}

The integral of squared error (ISE) is a commonly used performance evaluation index since it takes into account both overshoots and settling times; ISE is defined as:

$$ISE = \int_0^t (y - y_{sp})^2 dt \quad (7)$$

The comparison between the performances of MPC and PI control in terms of ISE is shown in Table 7. Obviously, MPC performs better than PI

strategy in maintaining product purities, resulting in lower values of ISE. It is worth noting that the performance of MPC is not always better than that of PI control, especially for the control of y_C . This can be explained by Eq. (4). The weighted sum of squared errors of controlled variables is optimized to be as small as possible. The summation of the ISE for all the controlled variables could be smaller than that of PI control, but this cannot assure that the ISE for each of the controlled variables is smaller than that of PI control. MPC may sacrifice the control qualities of certain variables to achieve an optimum overall performance.

**Fig. 16.** MPC vs. PI for temperature inferential control: dynamic responses of controlled variables to $\pm 10\%$ feed flow rate disturbances.

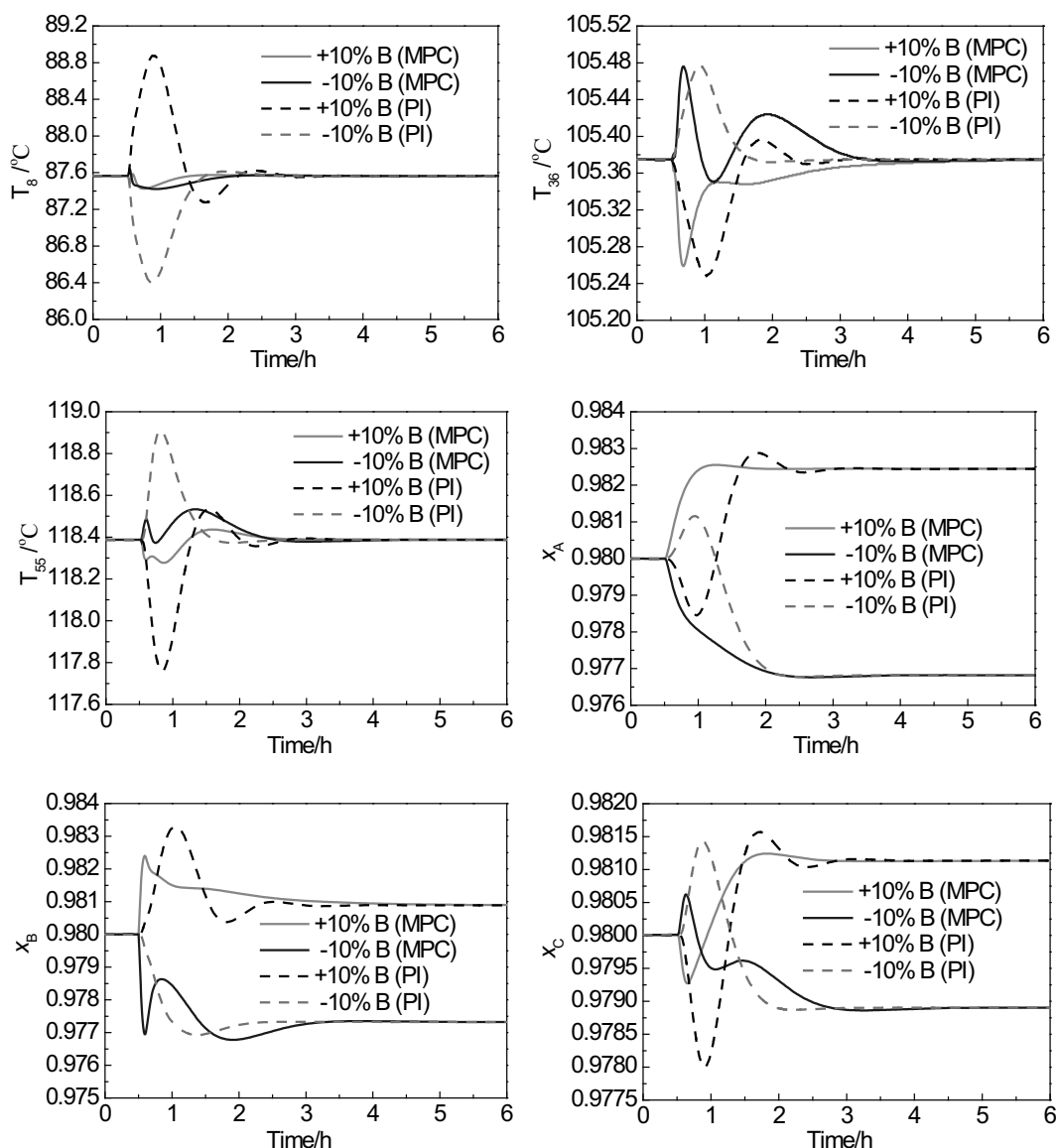


Fig. 17. MPC vs. PI for temperature inferential control: dynamic responses to $\pm 10\%$ feed composition of *n*-propanol disturbances.

4.2. Temperature inferential control

Figs. 16 and 17 show the dynamic responses of MPC vs. those of PI scheme for temperature inferential control in case of disturbances in feed flow rate and feed composition of *n*-propanol. Table 8 shows the comparison between the performances of MPC and PI control in terms of ISE. Despite that the control qualities of MPC for certain variables are not always better than that of PI control, the overall performance of MPC is generally better than that of PI control, which can be justified

by the summation of the ISE for the three controlled temperatures shown in Table 8. Although the three controlled temperatures can settle down quickly at their corresponding set points, three product purities cannot return to the designed values. Table 9 shows the new steady state values for product purities in case of disturbances in feed flow rate and feed composition. The product purity deviations exist even for the disturbances in feed flow rate. The maximum deviation of 0.78% occurs for the side stream purity in case of -10% feed flow rate disturbance. This can be explained by Fig. 18. When the feed flow rate

Table 8

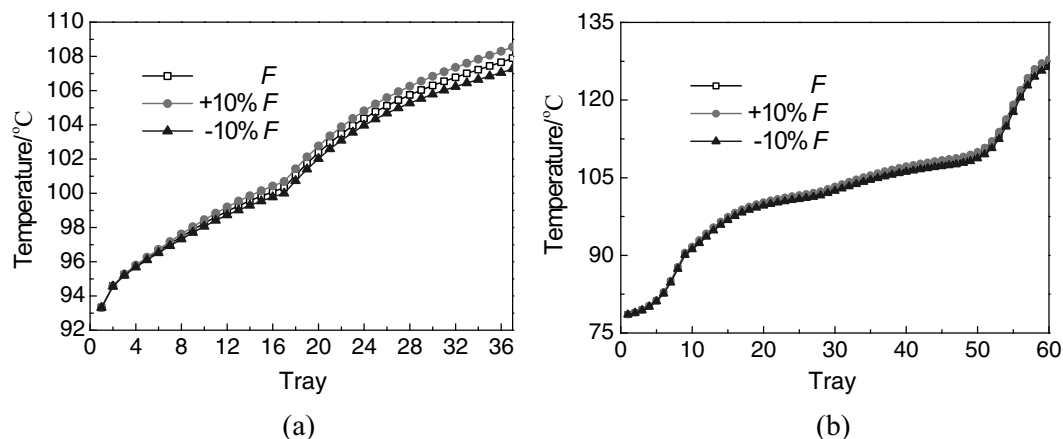
Comparison of the performance of MPC vs. PI control for temperature inferential control in terms of ISE

Disturbance	T_{8_PI}	T_{8_MPC}	T_{36_PI}	T_{36_MPC}	T_{55_PI}	T_{55_MPC}	Summation (PI)	Summation (MPC)
+10% F	0.4319	0.0014	0.0092	0.0066	0.1638	0.0195	0.6049	0.0275
-10% F	0.5874	9.79×10^{-4}	0.0089	0.0086	0.2165	0.0106	0.8128	0.0202
+10% A	0.0639	0.0015	3.44×10^{-4}	1.97×10^{-4}	0.0140	1.72×10^{-4}	0.0782	0.0019
-10% A	0.0597	0.0024	3.77×10^{-4}	2.52×10^{-4}	0.0137	1.57×10^{-4}	0.0737	0.0028
+10% B	0.7125	0.0062	0.0072	0.0036	0.1302	0.0059	0.8499	0.0158
-10% B	0.5844	0.0137	0.0042	0.0037	0.0913	0.0150	0.6799	0.0324
+10% C	0.0237	3.13×10^{-4}	3.06×10^{-4}	0.0011	0.0032	0.00406	0.0272	0.0054
-10% C	0.0201	2.90×10^{-4}	4.08×10^{-4}	7.68×10^{-4}	0.0023	9.65×10^{-4}	0.0230	0.0020

Table 9

New steady state values for product purities

Disturbance	+ 10% F	− 10% F	+ 10% A	− 10% A	+ 10% B	− 10% B	+ 10% C	− 10% C
x_A	0.9812	0.9787	0.9783	0.9815	0.9825	0.9768	0.9802	0.9797
x_B	0.9848	0.9722	0.9792	0.9805	0.9809	0.9773	0.9793	0.9796
x_C	0.9757	0.9835	0.9806	0.9794	0.9811	0.9789	0.9789	0.9812

**Fig. 18.** Temperature profiles of (a) prefractionator and (b) main column for $\pm 10\%$ feed flow rate disturbances with product purities equal to 98 mol%.

changes, as mentioned earlier, the pressure in the column will also change. Since the temperature at each tray varies with the pressure, simply controlling the temperatures of sensitive trays will inevitably lead to the deviations of the product purities from designed values. Given that the temperatures at all trays are affected by the pressure in the same way, differential temperature control may compensate for the temperature variations and reduce the deviations of product purities. The derivation of an effective differential temperature control scheme requires a detailed quantitative analysis of the DWC. This will be discussed in our future work.

5. Conclusions

In this article, a composition control structure and a temperature inferential control structure based on MPC strategies as well as their equivalent PI strategies are proposed for the control of a DWC for separating ethanol, *n*-propanol and *n*-butanol. Dynamic process is fully pressure-driven. GA is used for the weight tuning of MPC to obtain an optimized solution. The simulation results show that the linear MPC generally delivers an improved performance in stabilizing the nonlinear DWC flow sheet in case of disturbances in feed flow rate and feed composition, featured with reduced overshoots and less oscillation. For the composition control based on MPC scheme, directly controlling the content of *n*-butanol at the top of the prefractionator will cause the instability of the process. This is mainly due to the difference between the linear model and the nonlinear process. Despite that controlling the summation of the content of ethanol and *n*-propanol at the top of the prefractionator can successfully maintain stable on-specification operation in face of disturbances, the nonlinear model predictive control still deserves further investigation, especially for the control of highly nonlinear process.

Temperature measurement can guarantee an affordable cost and a shorter response time in comparison to on-line analyzers. However, simply controlling the temperatures on the sensitivity trays has difficulty achieving a tight control of the product purities for a ternary system. The future work will focus on enhancing composition inference capabilities through differential temperature control.

Nomenclature

B	bottoms flow rate
D	distillate flow rate
F	feed flow rate
K_C	proportional gain
L	reflux rate
L_1	liquid to the prefractionator
L_2	liquid from the prefractionator
L_{B1}	the sump level of the prefractionator
L_{B2}	the sump level of the main column
L_{D2}	liquid level in the reflux drum
MC	the main column
m_1	brake power of the compressor C_1
m_2	valve position that affects L_2
m_3	valve position that affects D
m_4	valve position that affects S
m_5	valve position that affects B
PC	the prefractionator
P_1	top stage pressure of the prefractionator
P_2	top stage pressure of the main column
Q_C	condenser duty
Q_R	reboiler duty
S	side stream flow rate
T_8	temperature of tray 8 in the main column
T_{36}	temperature of tray 36 in the main column
T_{55}	temperature of tray 55 in the main column
V_1	vapor from the prefractionator
V_2	vapor to the prefractionator
x_A	mole fraction of ethanol in the distillate
x_B	mole fraction of <i>n</i> -propanol in the side stream
x_C	mole fraction of <i>n</i> -butanol in the bottom product
y_{A+B}	mole fraction of ethanol and <i>n</i> -propanol at the top of the prefractionator
y_C	mole fraction of <i>n</i> -butanol at the top of the prefractionator
β_L	liquid split ratio
β_V	vapor split ratio
τ_I	integral time

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