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Multivariable model predictive control design of reactive distillation column for Dimethyl Ether production

A Wahid[1,2] and I G E P Putra[1]
[1] Chemical Engineering Department, Universitas Indonesia, Depok, Indonesia

E-mail: wahid@che.ui.ac.id; i.gede34@ui.ac.id

Abstract. Dimethyl ether (DME) as an alternative clean energy has attracted a growing attention in the recent years. DME production via reactive distillation has potential for capital cost and energy requirement savings. However, combination of reaction and distillation on a single column makes reactive distillation process a very complex multivariable system with high non-linearity of process and strong interaction between process variables. This study investigates a multivariable model predictive control (MPC) based on two-point temperature control strategy for the DME reactive distillation column to maintain the purities of both product streams. The process model is estimated by a first order plus dead time model. The DME and water purity is maintained by controlling a stage temperature in rectifying and stripping section, respectively. The result shows that the model predictive controller performed faster responses compared to conventional PI controller that are showed by the smaller ISE values. In addition, the MPC controller is able to handle the loop interactions well.

1. Introduction

Dimethyl ether (DME) is a simple ether which is widely used as propellant. It is also well-known as an excellent alternative diesel fuel which has high cetane number with lower NO_x, CO, and particulate emission [1]. Physical properties of DME are similar to liquefied petroleum gas (LPG), DME may hence be used as an alternative of LPG for domestic applications. In addition, DME is a key intermediate of other important chemical, such as dimethyl sulphate, methyl acetate, and light olefins. Due to its wide range of applications, the large scale production of DME is now required [2].

Currently, DME is produced via methanol dehydration in a catalytic fixed-bed reactor, followed by purification of DME in a sequence of two distillation columns [3]. Methanol dehydration in the conventional fixed-bed reactor is an equilibrium-controlled reaction, so that methanol conversion is limited that led the reactor to be operated at a high recycle rate which requires larger capital investment and operating costs [1,2]. This conventional process is costly in terms of operating cost, caused by the energy needed by two distillation columns. A single reactive distillation column can be used to reduced capital and operating cost, instead of one reactor followed by two distillation columns [4]. Bildea et.al. [5] stated that DME production through reactive distillation process led to savings of 30% in capital cost and 6% in energy requirement compared to conventional DME process for the same production rate.

While reactive distillation can have benefit over the conventional process, combination of reaction and distillation on a single column makes reactive distillation process a very complex system with

[2] To whom any correspondence should be addressed.

multiple steady state, high non-linearity of process, and strong interaction between process variables [6]. Wahid and Saputro [4] demonstrated the method of determining control structure of reactive distillation column for DME production. They used sensitivity and rangeability analysis to select a stage temperature as inferred variable to control DME product purity and its corresponding manipulated variable (MV). In these study, they successfully implemented a single-point PI control structure with a stage temperature at rectifying section as controlled variable (CV) and reboiler duty as MV, while the reflux ratio is controlled with ratio control.

Single-point control structure has an advantage on its less loop interaction [7]. However, in the single-point control structure which was proposed by Wahid and Saputro [4], no adjustment is made to control the stripping zone temperature. Therefore, the bottom purity is not controlled. The two-point control structure can maintain both product purities, but it led to strong interaction between CV and MV [6]. This study is focused on the implementation of multivariable model predictive control (MPC) to a reactive distillation column for the DME production based on two-point control structure. Both product purities are maintained by controlling the temperature of two stages which are selected by singular value decomposition (SVD) and rangeability analysis. Dynamic model of the process for the MPC controller is estimated by first order plus dead time (FOPDT) model.

2. Process Simulation

2.1. Reaction kinetics and thermodynamic properties

DME is produced from the methanol dehydration reaction in the liquid phase over an acid-base catalyst. To simplify the simulation, the kinetic for methanol dehydration to DME over ion exchange was modelled by simple power rate law in equation 1 and 2 [2].

$$r'_{\mathrm{DME}} = k'[\mathrm{MeOH}]^m[\mathrm{H_2O}]^n \tag{1}$$

$$k' = A'_0 \exp\left(-\frac{E'_a}{RT}\right) \tag{2}$$

The NRTL model was selected for the liquid phase properties calculation. The vapour phase properties calculated using RK equation of state. There is no azeotrope in the methanol–DME–water system [8].

2.2. Reactive distillation column

Rigorous simulation of the reactive distillation was performed in UniSim Design simulator. A reactive distillation column with capacity of 100,000 tonnes per year DME consist of 7 rectifying stages, 34 reactive stages, and 11 stripping stages [5] was used as base case for this work.

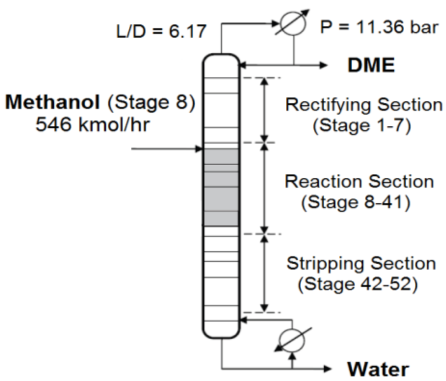

Figure 1. Schematic diagram of reactive distillation for the base case steady-state condition.

2.3. Model predictive control

In this study, a simple FOPDT process model was implemented in a 2 × 2 MPC controller built in UniSim Design. A series of step changes in reflux flow rate and reboiler duty were applied to generate input-output dynamic data. These data were then used to develop the FOPDT process model empirically using Method II [9].

3. Steady-state analysis

3.1. SVD analysis

The primary objective of reactive distillation control is to maintain product quality at its desired value. However, due to a large dead time and high price and maintenance cost, very few distillation columns use online composition analyser. Temperatures are widely used as inferential variable to control composition [10]. The two stages temperatures were selected by Singular Value Decomposition (SVD) analysis [11]. SVD analysis suggest that the stage 5 temperature should be controlled by the reflux flow rate (L) and the stage 47 temperature should be controlled by reboiler duty (Q_r).

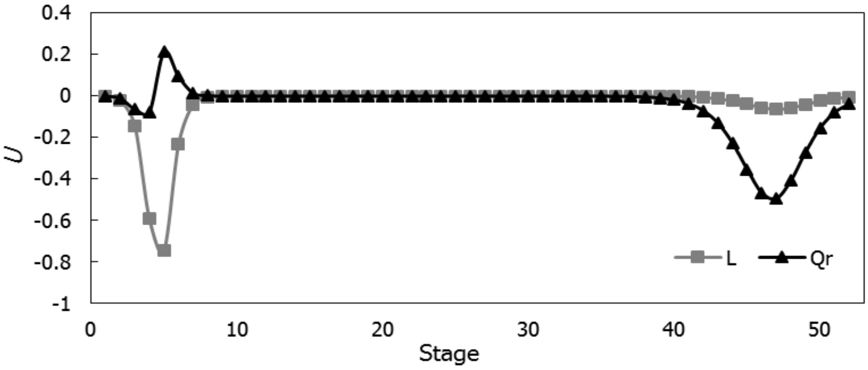

Figure 2. SVD analysis plot.

3.2. Rangeability analysis

Reactive distillation is highly nonlinear and possibly showing input multiplicity behaviour, thus the most sensitive input may have bad rangeability. So, this makes compromise between sensitivity and rangeability is needed for reactive distillation control structure design [4]. The steady-state variation of the sensitive tray temperatures obtained from SVD analysis as the two inputs are varied from its base case is studied in rangeability analysis. These input-output relations are plotted in Figure 3. The 5th and 47th stages temperatures did not show any input multiplicity for the its input variation. This makes 5th and 47th stages temperatures can be the output (CV) and can be paired with its corresponding inputs (MV).

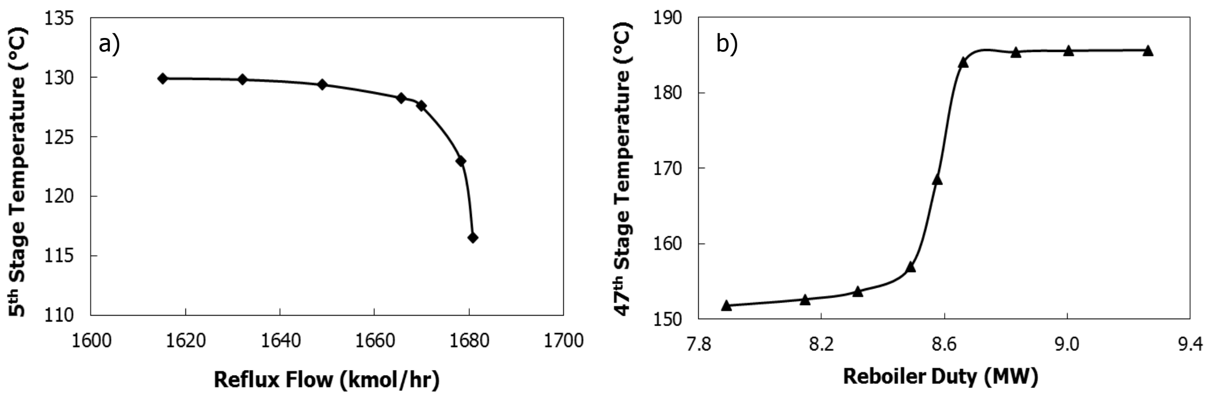

Figure 3. Steady-state input-output relation of a) reflux flow rate to stage 5 temperature, b) reboiler duty to stage 47 temperature.

4. Controller design

4.1. Controller configuration

Figure 4 shows the PI and MPC controller configurations. In the MPC configuration, the stages 5 and 47 temperatures are controlled with the reflux flow rate and the reboiler heat duty in a two-input two-output system. In the two-point PI configuration, the stage 5 temperature is controlled using the reflux flow rate and the stage 47 temperature is controlled using the reboiler duty. As the comparison, this work also investigates the performance of a single-point PI configuration that was proposed by Wahid and Saputro [4]. Temperature at the stage 5 which is the most sensitive stage to the change in reboiler duty, is controlled by reboiler heat duty, while the reflux ratio is controlled by distillate flow rate. The column inventory are controlled by three single-loop PI controllers. The column pressure is controlled by condenser duty and the reboiler level is controlled by bottom flow rate. In the MPC and two-point PI configurations, condenser accumulator level is controlled by distillate flow rate, while in the single-point configuration, condenser accumulator level is controlled by reflux flow rate.

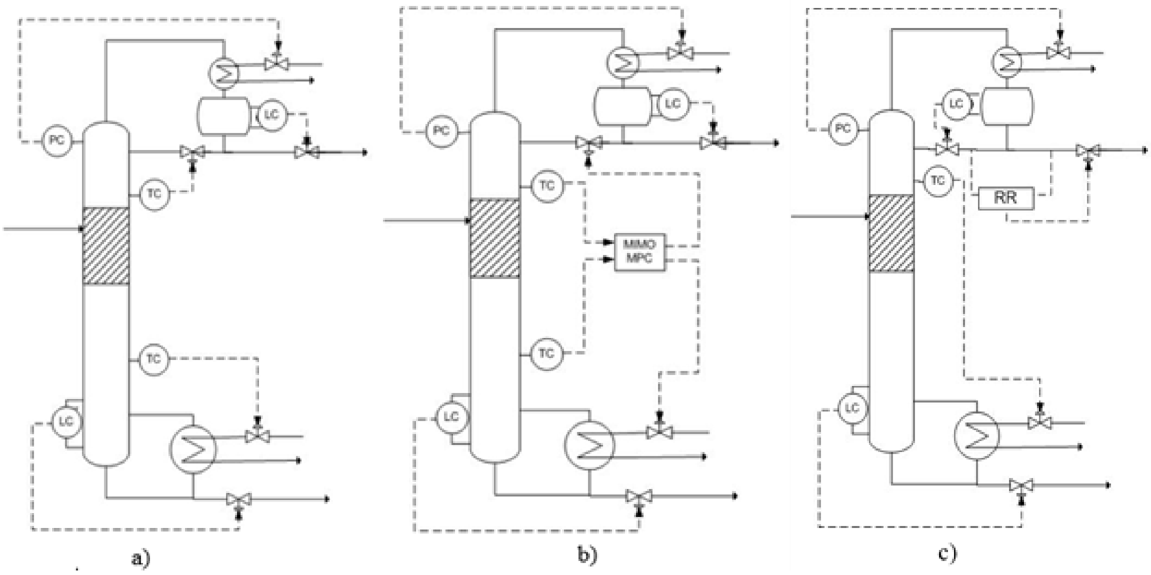

Figure 4. a) Two-point PI control configuration, b) MPC control configuration, c) Single-point PI control configuration.

4.2. Process model identification

In this study, dynamic model of reactive distillation column was modeled as a simple FOPDT model. Model identification was done by changing reflux flow rate and reboiler duty in a step test to generate input-output dynamic data. Table 1 summarizes the obtained transfer functions explaining the relationships of the two inputs (i.e. reflux flow rate and reboiler duty) and the two outputs (stages 5 and 47 temperatures). The units for all time constants are minutes. These model was implemented for the MPC controller.

Table 1. Transfer functions for the process models of DME reactive distillation.

	L	Q_r
T_5	$\frac{-6.912e^{-0.035s}}{0.272s+1}$	$\frac{1.030e^{-0.077s}}{0.185s+1}$
T_{47}	$\frac{-0.537e^{-0.89s}}{0.421s+1}$	$\frac{3.351e^{-0.102s}}{0.627s+1}$

4.3. Controller parameter

The two PI controllers were then tuned by using Tyreus-Luyben method, while the MPC controller was tuned by fine tuning. Tables 2 and 3 summarize the controller parameters.

Table 2. Single-point and two-point PI controllers parameters.

Controller	Single-point PI		Two-point PI	
	K_c	T_i (min)	K_c	T_i (min)
Stage 5 temperature	0.921	0.251	0.853	0.145
Stage 47 temperature	-	-	0.055	0.054
Reflux ratio	0.500	0.500	-	-
Column pressure	0.829	0.273	0.829	0.273
Condenser level	1.018	0	1.121	0
Reboiler level	2.450	0	2.450	0

Table 3. MPC controller parameters.

Controller	K_c	T_i (min)	P	M	T
Stages 5 and 47 temperatures	-	-	23	2	1
Pressure column	0.829	0.273	-	-	-
Condenser level	1.121	0	-	-	-
Reboiler level	2.450	0	-	-	-

5. Results and discussion

5.1. Stage 5 temperature control

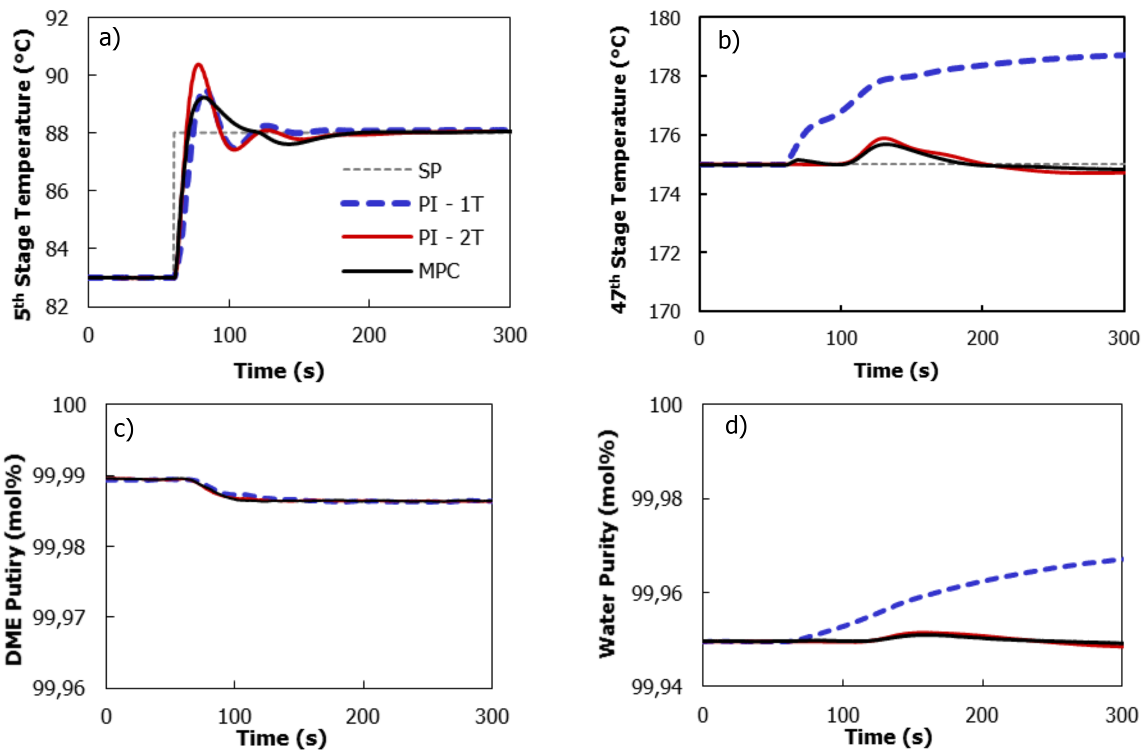

Figure 5. Dynamic responses to a change in stage 5 temperature set-point: a) stage 5 temperature, b) stage 47 temperature, c) DME purity, d) water purity.

Figure 5a shows the dynamic responses in case of the set-point change in stage 5 temperature. The multivariable MPC and single-point PI controllers perform responses with smaller overshoot compared to the response of two-point PI controller. Figure 5b shows the effect of the stage 5 temperature set-point change on the dynamic responses of the stage 47 temperature controller. MPC controller performs the best responses in overcoming the interaction between the stages 5 and 47 temperature control loops. Compared to the two-point PI controller, the single-point PI controller is a better in overcoming the loop interaction because in the single-point PI controller there is only one closed loop to control the temperature. Top and bottom product compositions can be controlled through temperature control of stages 5 and 47 as shown in Figures 5c and 5d. The purity of DME decreases when there is a positive change in stage 5 temperature set-point. The single-point PI controller can not maintain the bottom product because of the uncontrolled stage 47 temperature.

5.2. Stage 47 temperature control

Figure 6b shows that the response of the MPC controller is faster and more stable under a change in the stage 47 temperature set-point. In addition, the undershoot generated by the MPC controller is smaller than the two-point PI controller. A step change in the set-point of the stage 47 temperature causes a disturbance effect on the stage 5 temperature control loop which can be seen from the stage 5 temperature deviation from the set-point as shown in Figure 6a. MPC controller can minimize the disturbance effect on stage 5 temperature and overcome the loop interactions. The purity of the bottom product decreases when there is a decrease in the stage 47 temperature set-point.

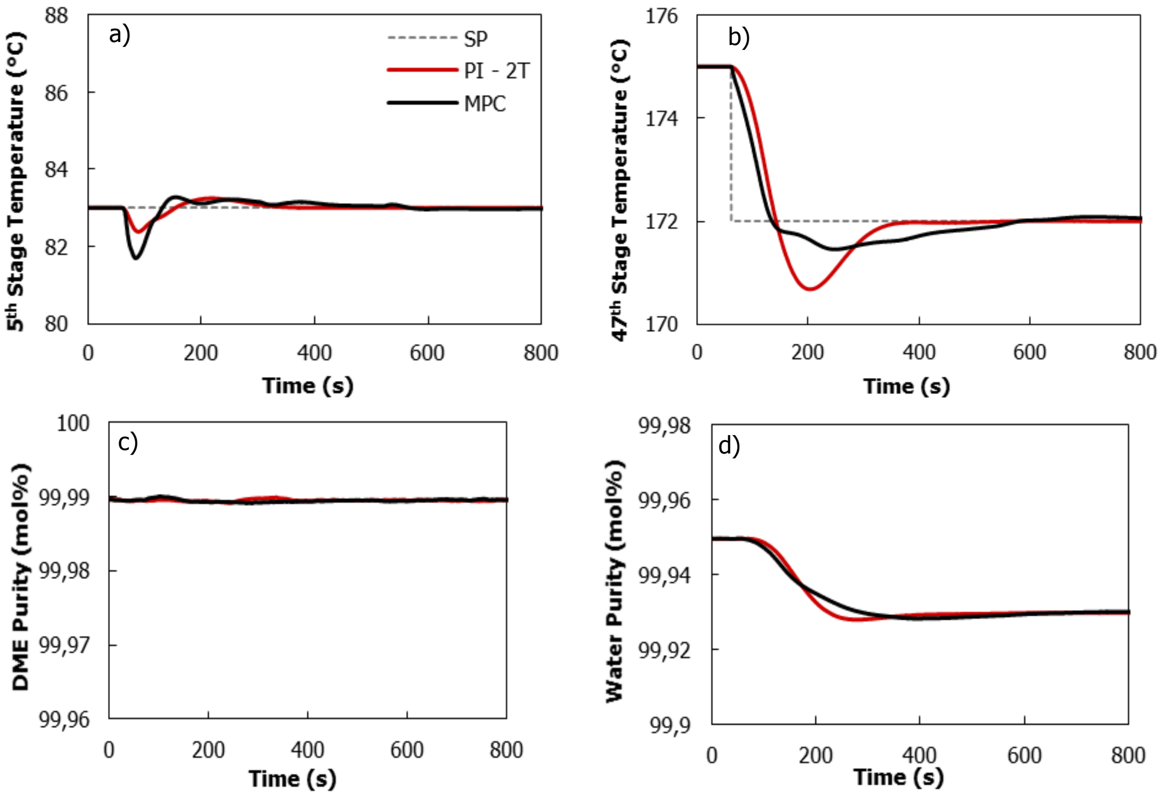

Figure 6. Dynamic responses for to a change in stage 47 temperature set-point: a) stage 5 temperature, b) stage 47 temperature, c) DME purity, d) water purity.

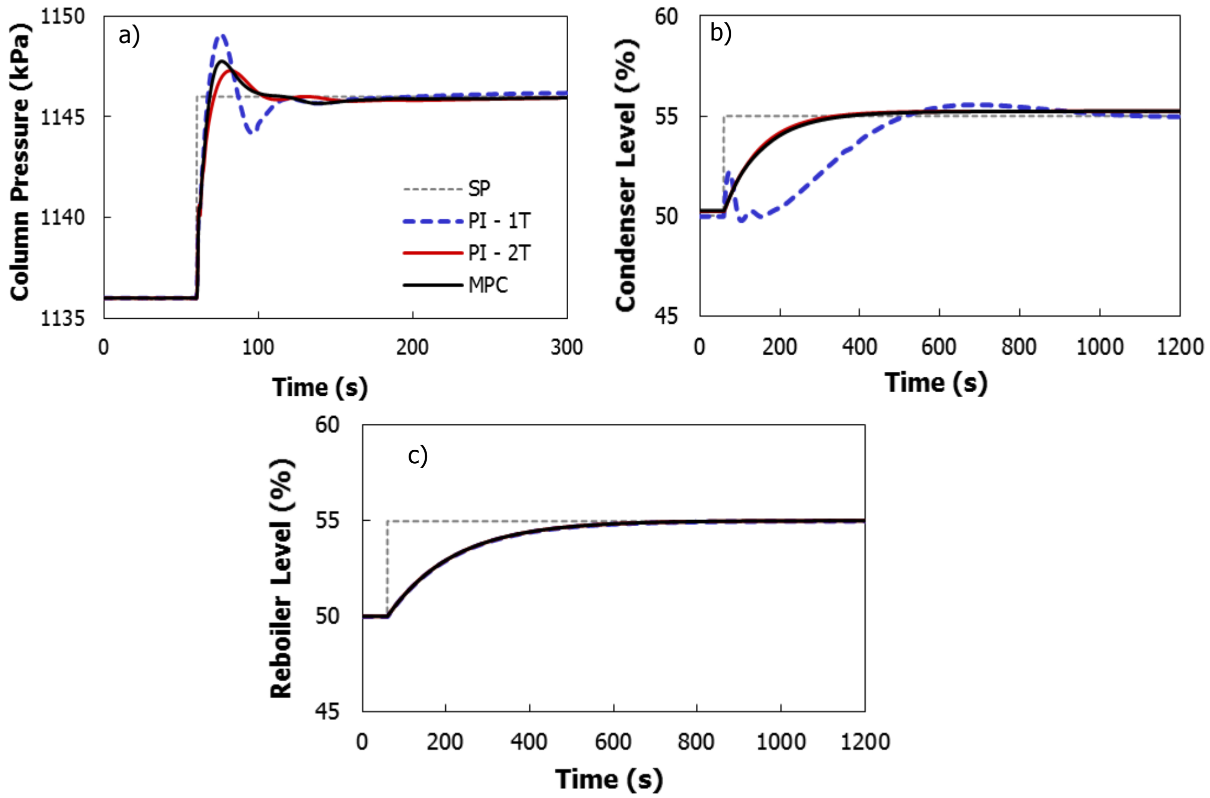

Figure 7. Dynamic responses to a change in the set-point of a) top column pressure, b) condenser accumulator level, c) reboiler level.

5.3. Pressure control

The dynamic responses of pressure controllers under a change in its set-point are shown in Figure 7a. The rise time of the two-point PI and multivariable MPC responses are slightly slower than the single-point PI controller responses. However, the responses of the MPC and two-point PI are more stable with small overshoot.

5.4. Condenser level control

The dynamic responses of the two-point PI and multivariable MPC controller are similar because it use the same configuration and tuning parameters. In the two-point PI and MPC controllers, the condenser accumulator level is controlled by adjusting the distillate flow rate. The dynamic response of the single-point PI controller is different to the other two configurations. In the single-point PI control configuration, there is interaction between the condenser level control and stage 5 temperature control loops. When there is a change in level set-point, the controller initially decreases reflux flow rate to increase the condenser accumulator level. As a consequence, the stage 5 temperature increase, then the stage 5 temperature controller adjusts reboiler duty that makes the vapour flow rate change. The interaction between the condenser level control and stage 5 temperature control loops is shown by the oscillatory response in the Figure 7b.

5.5. Reboiler level control

The three controllers use the same configuration and tuning parameters for the reboiler level control. The dynamic responses of the three controllers show its similar behaviour. Figure 7c shows that there is no interaction between the reboiler level control with the other control loops.

Table 4 shows the ISE (Integral of Squared Error) value of each controller in case of set point tracking. The smaller the ISE value, the better the performance of the controller. Overall, the multivariable MPC controller performs fastest responses with smaller ISE values and less oscillation under set-point step changes. Two-point PI control provides better control performances compared to single-point PI control, regarding to its ability to maintain the stage 47 temperature and the bottom product purity.

Table 4. ISE values in the case of set point tracking.

Controller	Single-point PI	Two-point PI	MPC
Stage 5 temperature	186.0	178.0	134.9
Stage 47 temperature	Uncontrolled	504.0	280.8
Column pressure	301.3	185.5	197.6
Condenser level	4983.0	1000.1	1003.3
Reboiler level	1983.6	1986.8	1986.7

6. Conclusions

In this article, we shown that the controllers with two-point control structure (i.e. two-point PI and multivariable MPC) provide better control performance for DME reactive distillation column, compared to the single-point control structure. The two-point control structures can control both product purity, while the single-point control structure can only control top product purity. The stage 5 temperature in rectifying zone which infers top product purity, is controlled using reflux flow rate and the stage 47 temperature in stripping zone which infers bottom product purity, is controlled using reboiler duty. The multivariable MPC controller performs better responses than the PI controllers as shown by its smaller ISE values. In addition, the multivariable MPC controller is able to handle the loop interactions well.

Acknowledgments

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