Optimal Policy Tracking of a Batch Reactive Distillation by Neural Network-based Model Predictive Control (NNMPC) Strategy

Kwantip Konakom, Paisan Kittisupakorn, Aritsara Saengchan, and Iqbal M. Mujtaba

***Abstract*—This paper presents the use of neural network-based model predictive control (NNMPC) for handling predefined optimal policy tracking determined by dynamic optimization strategy of a batch reactive distillation column. Multi-layer feedforward neural network model and estimator are developed and used in the model predictive control algorithm. The results show that the NNMPC provides satisfactory control performance for set point tracking problems. The robustness of the NNMPC is investigated with respect to plant/model mismatches and compared to a conventional proportional controller (P). It has been found that the NNMPC provides better control performance than the P controller does in all cases.**

***Index Terms*— batch reactive distillation, model predictive control, neural network, plant/model mismatches.**

I. Introduction

Batch reactive distillation, integrating reaction and separation into a single stage, offers many benefits as well as the possibility to overcome restrictions given by chemical reaction equilibrium. Reduced capital cost, higher conversion, improved selectivity and lower energy consumption are a few of the potential advantages offered by a batch reactive distillation column.

Research on various aspects of a batch reactive distillation column such as process synthesis, modeling, simulation, optimization and control etc., has been in progress. However, there have been few papers published on the controller design of the batch reactive distillation column. An artificial neural network estimator to provide estimates of product compositions to be used in an inferential control algorithm was proposed [1]. State estimator and generic model controller was developed [2], [3]. Monroy-Loperena and Alvarez-Ramirez [4] used an output-feedback controller (PID), whereas Sorensen *et al.* [5] proposed an optimal control and on-line operation.

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In recent years, an artificial neural network-based model predictive control has successfully exhibited excellent control performance even through the presence of model/plant uncertainties. Neural networks are often used in many control configurations and can be applied in various chemical process plants because it offers a promising improvement of process modeling and control of nonlinear and complex systems. For example, Kittisupakorn *et al.* [6] proposed the NNMPC for controlling a steel picking process; Engell and Fernholz [7] proposed the NNMPC for controlling of a semi-batch reactive distillation process; and Filet *et al.* [8] developed the model predictive control based on a non-linear nonparametric dynamic system model—the dynamic neural network of a ternary batch distillation process.

Therefore, the objective of this work is to design a neural network based-model predictive controller for tracking the predefined optimal reflux ratio policy of a batch reactive distillation column. In practice, distillate composition at current time, needed as one of the NNMPC inputs, is not available. Hence, a neural network-based estimator is also developed to estimate current distillate composition from available measured compositions with delays. The robustness of the proposed controller is evaluated and compared to the conventional P controller in the presence of plant/model mismatches: kinetic rate and vapor-liquid equilibrium constants.

This paper is divided into five sections. A process description and a determination of the optimal reflux policy are presented in section II and III, respectively. The proposed NNMPC structure consisting of a neural network (NN) estimator and a neural network model is described in section IV, whereas the performance of the proposed controller compared with a conventional P controller is investigated in section V and a conclusion is presented in the last section.

II. Process Description

A batch reactive distillation column to produce the ethyl acetate studied in this work as shown in Fig. 1. consists of 10 stages; the first stage is the total condenser and the tenth stage is the reboiler. Information regarding the column configuration, feed, feed composition, column holdup, etc., is given in Table I.

A chemical reaction occurred in the column in liquid phase produces ethyl acetate as a main product and water by the esterification of ethanol with acetic acid:

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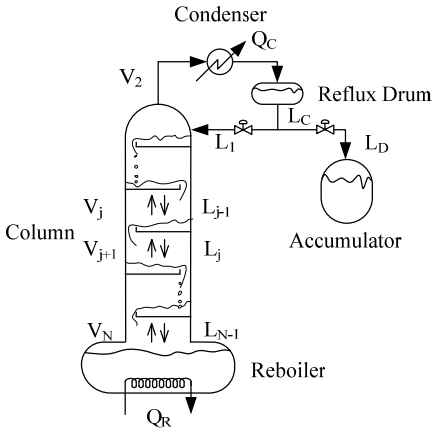

Fig. 1. Conventional batch reactive distillation [10]

Table I. Column specifications

System: Acetic acid/ethanol/ethyl acetate/water	
Total feed charge, H_{10}:	5.0 *kmol*
Feed composition (mole fraction):	0.45/0.45/0.0/0.1
Column holdup	
Reflux drum holdup:	0.1 *kmol*
Internal plates:	0.0125 *kmol*
Heat supplied to the reboiler, Q_R:	50 *MJ / hr*
Column pressure:	1.013 *bar*

Table II. Vapor-liquid equilibrium and kinetic data for ethanol esterification [9]

Vapor-Liquid Equilibrium:

$K_{j,1} = 2.25\times10^{-2}T_j - 7.812, \quad T_j > 347.6\ K$

$K_{j,1} = 0.001, \quad T_j \le 347.6\ K$

$\log K_{j,2} = (-2.3\times10^{3})/T_j + 6.588$

$\log K_{j,3} = (-2.3\times10^{3})/T_j + 6.742$

$\log K_{j,4} = (-2.3\times10^{3})/T_j + 6.484$

Kinetic data:

Rate of reaction, $gmol/(L\cdot min)$; $r = k_1C_1C_2 - k_2C_3C_4$

where rate constants are $k_1 = 4.76\times10^{-4}$ and $k_2 = 1.63\times10^{-4}\ L/(gmol\cdot min)$, and C_i stands for concentration in $gmol/L$ for the i^{th} component

	acetic acid + *ethanol* ⇔ *ethyl acetate* + *water*			
	(1)	(2)	(3)	(4)
Boiling point (K)	391.1	351.5	350.3	373.2

For the ethanol esterification reaction, the vapor-liquid equilibrium and kinetic data presented in Mujtaba and Macchietto [9] are listed in Table II.

III. Optimal Reflux Ratio Policy

In this work, the optimal reflux ratio profiles are determined by maximizing the amount of distillate product subject to the process model, product specification and a given batch time. Details of the mathematical model of the batch reactive distillation column are described in Konakom *et al.* [10]. In this paper, the purity of the distillate product is specified by 90.0% by mole of ethyl acetate and the operating batch time is fixed at 8 hrs.

Mathematically, the optimization problem of the column can be written as:

$$\underset{R_f(t)}{Max} \quad J$$

subject to $x_{a,3}(t_f) \ge 0.90$

mathematical model of the column

with initial conditions

$0.51 \le R_f(t) \le 1.0$

$Q_R = 50\ MJ/hr$

$t_f = 8\ hrs$

where J is the weight of the distillate product, $x_{a,3}(t_f)$ is the composition of the third component, ethyl acetate, in the accumulator at the end of the operation (t_f), $R_f(t)$ is the reflux ratio as a function of time (t). Details for solving this dynamic optimization problem are in Konakom *et al.* [10].

The optimal results show that the increase in the number of time intervals (or set point change) produces more distillate product as shown in Table III. The obtained optimal reflux profiles given in Fig. 2. show that the column is started-up under total reflux condition. Therefore, in this work, the controller is switched on when the total reflux operation is ended. The predefined set point, ethyl acetate composition in the distillate accumulator, can be calculated from the optimal reflux policy and will be used as the predefined set point in the next section. In this paper, the optimal reflux policy with 16 intervals is used as a case study for closed-loop studies.

Table III. Optimal results [10]

Number of interval	Distillate product (kg)	Product purity (mole fraction)
2	83.69	0.90
4	83.96	0.90
8	88.11	0.90
16	89.01	0.90

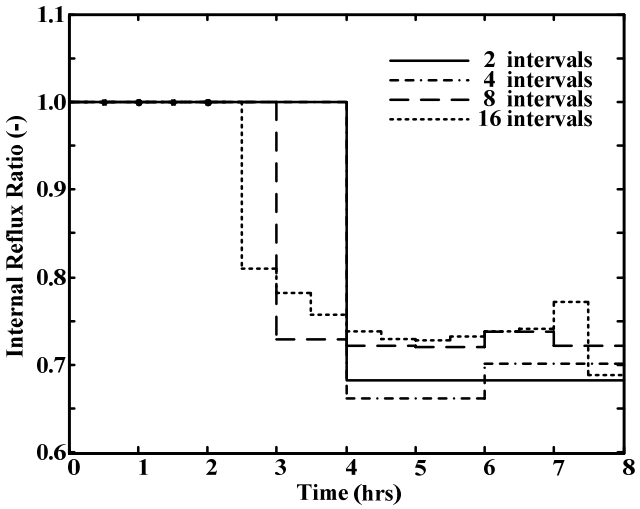

Fig. 2. Optimal reflux ratio profiles [10]

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IV. Neural Network-Based Model Predictive Control Strategy

This section is composed of 2 subsections. Section IV. *A.* presents the estimation of ethyl acetate distillate composition using a neural network based estimator, and Section IV. *B.* presents the modeling of neural network used as a model in the NNMPC algorithm. In both subsections, the neural networks are developed based on the simulation of the batch reactive distillation column. As described in the previous section, the controller is switched on after the total reflux operation is ended. The column is initially operated under total reflux for 2.5 hrs, and then the distillate is withdrawn to the accumulator. Consequently, to develop the neural networks, process data are collected during 2.5 and 8 hrs of the column batch time. The data sampling of 5.5 hrs is divided into 3 intervals and in each interval the process is simulated with the internal reflux ratio of 0.65 - 0.85 with a step of 0.02. Hence, in this work, 1,331 data patterns have been used to train the neural network model and neural network estimator. In each pattern, data are sampled every 2 minutes and randomly selected and grouped into 3 different sets: 111 data for training, 39 data for testing, and 15 data for validating. In this paper, multilayer feedforward networks have been used and trained by Levenberg-Marquardt back-propagation approach. The number of hidden layers is set to 1 and the maximum number of nodes in this layer is 10 in both networks. The hyperbolic tangent sigmoid and the linear are used as transfer functions of the hidden and output layers, respectively. Minimum mean squared error (MSE) is used as the criterion for the network selection and also for the stopping of weights and bias adjustment. The neural network training is switched between the train and test data and the training stops when the desired mean squared error (MSE) reaches the specified value of 10^{-6} for both cases.

However, it is noted that the effective use of the obtained neural networks is limited in the range of training. In this work, the neural network model is trained in the range of 0.65-0.85 of reflux ratio.

A. Neural Network-Based Estimator

From simulation results, it has been found that the optimum architecture of NN for the estimation of the ethyl acetate distillate composition consists of 4 input-nodes, 10 hidden-nodes and 1 output-node. The designed inputs are an ethyl acetate distillate composition at time *k-5* (with delay by 10 minutes), top-tray temperatures at time *k* and *k-1*, and an internal reflux ratio at time *k-1*, whereas the determined output is the ethyl acetate distillate composition at time *k*. The MSE of this architecture is equal to 4.42×10^{-8}.

B. Neural Network-Based Model Predictive Control

The neural network architecture to be used as the model in the predictive controller consists of 4 input-nodes, 9 hidden-nodes and 2 output-nodes. The network inputs are the ethyl acetate distillate composition at time *k* obtained from the estimator, top-tray temperatures at time *k* and *k-1*, and the internal reflux ratio at time *k*, whereas the network outputs are the ethyl acetate distillate composition and the top-tray temperature at time *k+1*. The MSE of this architecture is equal to 6.15×10^{-9}.

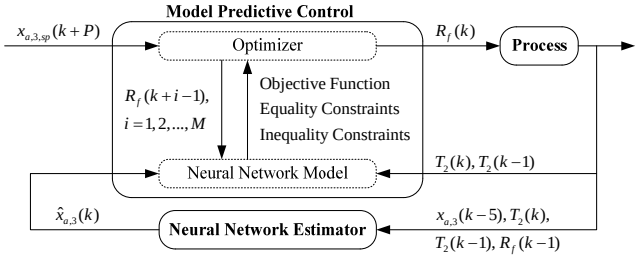

Fig. 3. The NNMPC integrating with NNE strategy

In this work, the reflux ratio profile (manipulated variable) can be determined by solving a minimization problem based on an objective function subject to the neural network model, product specification constraints, and lower and upper bounds of reflux ratio and the ethyl acetate distillate composition. Closed-loop control by the neural network model predictive control incorporating with neural network estimator is shown Fig. 3. The objective function in the NNMPC algorithm is to minimize errors between the predicted outputs and the set point values, and also the control moves evaluated over the prediction horizon (*P*) as described below.

$$\min_{Rf(k),\ldots,Rf(k+M-1)} \sum_{i=1}^{P}\left[W_1\left\{x_{a,3,sp}(k+i)-\hat{x}_{a,3}(k+i)\right\}^2+W_2\left\{\Delta R_f\right\}^2\right]$$

subject to neural network model described in section IV. *B.*

$$0.65 \le R_f \le 0.85$$

$$0.0 \le \hat{x}_{a,3} \le 1.0$$

$$\hat{x}_{a,3}(k+P) = x_{a,3,sp}(k+P)$$

To clearly describe on the NNMPC algorithm, Fig. 4. shows the data flow diagram in the neural network estimator and neural network model. Number in the circle, ◯, represents the measured value whereas number with hat in the gray-filled circle, ◉, represents the estimate. When the ethyl acetate distillate composition is estimated by the neural network-based estimator, it is then sent to the neural network model. At the first prediction, trial reflux ratio at time *k* is given to the model, and both ethyl acetate composition and top-tray temperatures at time *k+1* are estimated. These estimated values and trial reflux ratio at time *k+1* then work as inputs in the second prediction. After *M* steps prediction, the trial reflux ratio is kept constant and equal to the reflux ratio at time *k+M-1*. Until the P^{th} step of prediction, ethyl acetate composition and top-tray temperatures at time *k+P* are estimated. In this step, the product purity must satisfy the

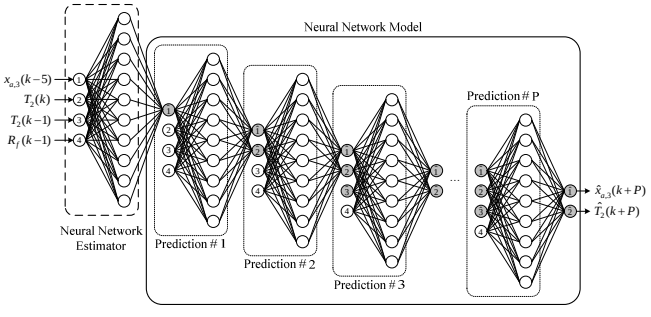

Fig. 4. Data flow diagram of the NN estimator and NN model

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used in NNMPC scheme

equality constraint—that is the estimated ethyl acetate composition must be equal to its predefined set point, $\hat{x}_{a,3}(k+P) = x_{a,3,sp}(k+P)$. If the predicted composition satisfies the set point, the optimization is then terminated, and the first value of the reflux ratio is applied to the process as shown in Fig. 3.

V. Simulation Results

The implementation of NNMPC with NN estimator to control the distillate product is demonstrated in this section. The performance of the NNMPC strategy for all tests is compared with that of conventional P controller. Tuning parameters of the conventional P and NNMPC algorithms are summarized in Table IV. All simulations studied are carried out on Window XP Professional 2002 (Core2 Duo 2.60 GHz) by optimization and neural network toolboxes in MATLAB program version 7.1.0.

First, the performance of the controllers is tested in nominal case where the model parameters are determined correctly. Fig. 5. shows the performance of the obtained NN estimator comparing the actual and NN-estimated values of the ethyl acetate distillate composition. It is found that the NN estimator provides an accurate prediction of the distillate composition but with some errors for the first hour. With this estimated composition, the NNMPC can give reasonably good distillation composition control with a small overshoot occurring at the beginning as shown in Fig. 6. (a). The overshoot of the control response occurs when the estimated composition, one of the inputs to the NNMPC, differs from the actual. After the first hour of the controller action, however, when the NN estimator gives more accurate estimates of the composition, the controller then calculates the reflux ratio correctly and therefore the distillate composition is kept on the predefined set point as shown in Fig. 6. (a). The smooth controller action, reflux ratio, is shown in Fig. 6. (b).

Fig. 7. shows the distillate product control by the conventional P controller in nominal case. It can be seen from Fig. 7. (a) that the distillate composition is slightly higher than the set point whereas the product amount is 1.30 kg lower than that is controlled by NNMMC as shown in Table V.

In the cases of plant/model mismatches, NNMPC and P controllers are tested without any changes in tuning parameters as shown in Table IV. In this work, the robustness of the controllers is tested by decreasing 20% of k_1 and increasing 20% of K_2 from their nominal values. The simulation results for all cases are given in Fig. 8. and Table V. It can be seen that the NNMPC drives the ethyl acetate distillate product to its predefined set point even if the reaction rate and vapor-liquid equilibrium constants are mismatched from the plant model. In these mismatch cases, the distillate product can be produced 86.66 and 71.47 kg,

Table IV. Tuning parameters of P and NNMPC algorithms

NNMPC controller			
W_1	= 5	W_2	= 10
M	= 5	P	= 10
P controller			
K_c	= 100		

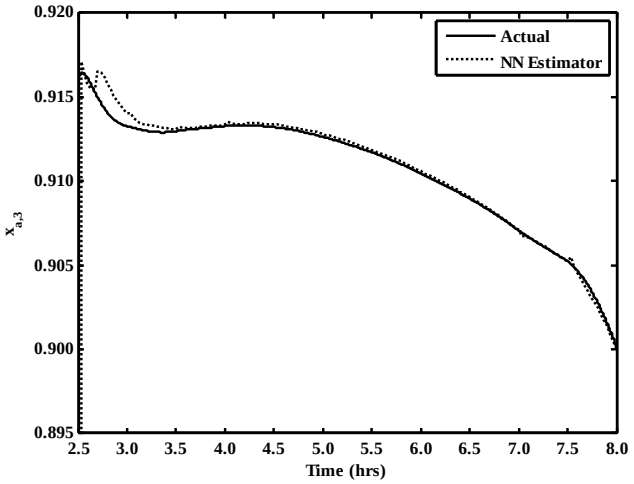
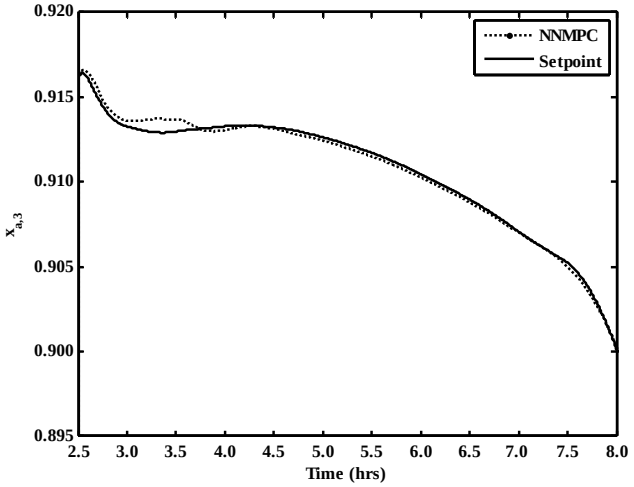
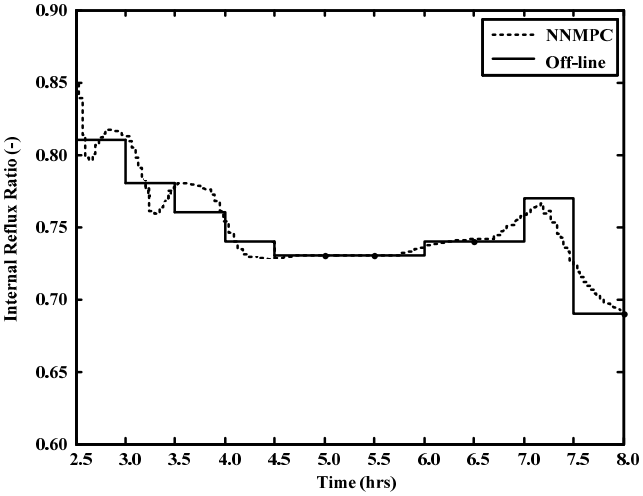


Fig. 5. Estimated ethyl acetate distillate composition



(a) Ethyl acetate distillate composition



(b) Reflux ratio

Fig. 6. Set point tracking with NNMPC in nominal case

respectively which are less than in the nominal case. The distillate product is still on-specification because the NNMPC drives the ethyl acetate distillate composition to its predefined set point in every iteration of control calculation. On the other hand, the conventional P controller cannot drive

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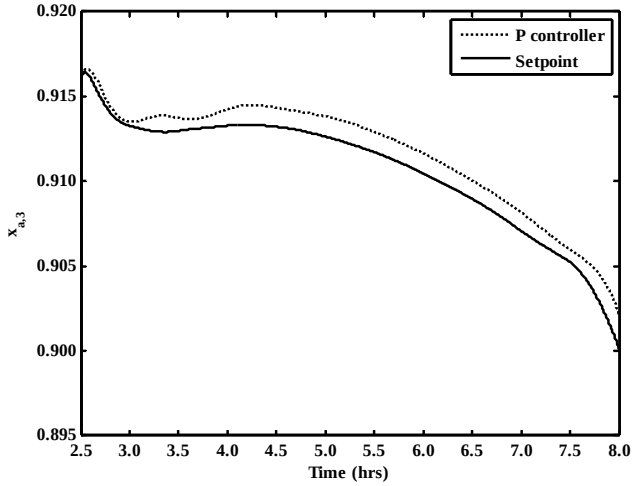
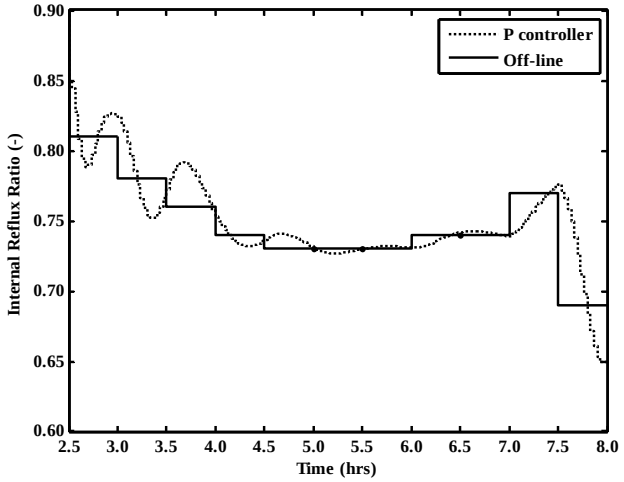
the product to its specification ($x_{a,3}(t_f) < 0.90$) even though the amount of distillate product is higher than that of NNMPC. The distillate in both mismatch cases is off-specification.



(a) Ethyl acetate distillate composition



(b) Reflux ratio

Fig. 7. Set point tracking with P control in nominal case

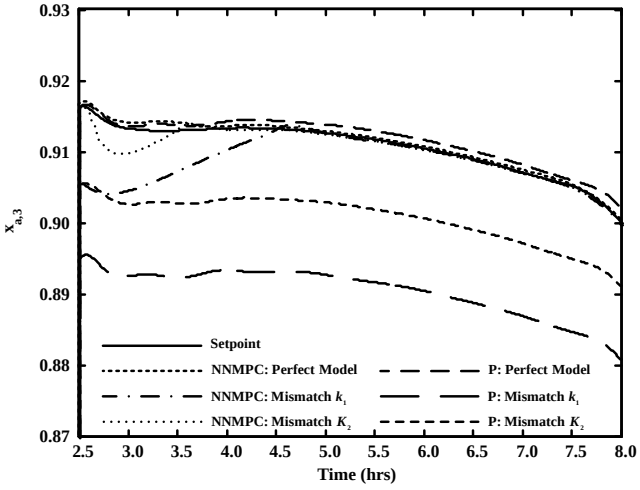


Fig. 8. Closed-loop performance of NNMPC compared with P control in all cases

Table V. Closed-loop performances of NNMPC and P control

Controller	*IAE*	$x_{a,3}(t_f)$	H_a (*kg*)
Perfect Model			
NNMPC	0.0013	0.90	88.77
P controller	0.0055	0.90	87.47
Mismatch k_1			
NNMPC	0.0139	0.90	80.02
P controller	0.1113	0.88	86.12
Mismatch K_2			
NNMPC	0.0031	0.90	88.66
P controller	0.0550	0.89	87.86

VI. Conclusion

The neural network-based model predictive control incorporating with the neural network-based estimator has been implemented to control the distillate product in the batch reactive distillation column. The NNMPC performance is compared with the performance of the conventional P controller. Simulation results show that both controllers give good control response in a nominal case. However, in the presence of plant/model mismatches in reaction rate and vapor-liquid equilibrium constants, the NNMPC is more robust than the conventional P controller. The NNMPC can maintain the distillate product purity on its specification whereas the conventional P controller lets the product out of specification in the presence of plant/model mismatches.

Acknowledgment

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