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Article

Neural Network Based Model Predictive Control of Batch Extractive Distillation Process for Improving Purity of Acetone

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Abstract. In a pharmaceutical industry, batch extractive distillation (BED), a combination process between extraction and distillation processes, has been widely implemented to separate waste solvent mixture of acetone-methanol because of minimum-boiling azeotrope properties. Normally, water is used as solvent and semi-continues mode is proposed to improve purity of acetone. The solvent is charged into the BED column with total reflux start-up until the purity of a desired product is achieved. After the total reflux start-up period is ended, a dynamic optimization strategy is applied to determine an acetone distillate composition profile maximizing the weight of the distillate product (acetone). The acetone distillate composition profile is used as the set point of neural network model-based controllers: the neural network direct inverse model control (NNDIC) and neural network based model predictive control (NNMPC) in order to achieve the acetone composition with the purity of 94.0% by mole within 9.5 hours. It has been found that although both NNDIC and proportional integral derivative (PID) control can maintain the distillate purity on its specification for the set point tracking and in presence of plant uncertainties, the NNMPC provides much more satisfactory control performance and gives the smoothest controller action without any fluctuation when compared to the NNDIC and PID.

Keywords: Batch extractive distillation, dynamic optimization, neural network based model predictive control, neural network direct inverse model control.

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1. Introduction

A waste solvent mixture of acetone-methanol water from a pharmaceutical plant, minimum boiling azeotrope property, is difficult to separate by conventional batch distillation. Consequently, to improve effectiveness of the batch distillation, the extraction and the distillation are combined into one column called a batch extractive distillation column. It provides a potentially very attractive alternative to increase large quantities of desired products separated immediately and continuously when the solvent is fed into the column. However, a batch extractive distillation process exhibits an inherent nonlinear dynamics and complex behavior. Operation and optimization of a batch extractive distillation process have been studied by few researchers. One literature has proposed the operation under constant reflux ratio and optimization of product's quantity and quality in a fixed time with respect to less quantity of solvent [1]. S.M. Milani [2] has presented the operation in the batch mode with optimized solvent feed rate to achieve maximum recovery of a high purity top product in the batch extractive distillation (BED) process. The optimization with maximum product and minimum time objective functions in the fashion of one or two time intervals are considered in both batch and semi-continuous modes [3]. In addition, the BED as a hybrid process [4] and the BED control using a rigorous dynamic simulation via Aspen DynamicsTM [5] have been studied.

Neural network is like human newborn where it needs to be developed, trained and taught to perform desired tasks. It captures the (highly nonlinear process) relationship between the inputs and the outputs of a true process with a considerably lower computational load than required by a mathematic model of the plant [6], [7], learns easily and requires little or no a priori knowledge of the structure [8], [9]. Neural network has been applied in neural network based modeling, optimization and control [10-13].

Model predictive control (MPC) is an optimal control based method to determine control action by minimizing a specified objective function. Since, constraints inclusion of MPC leads to tighter control and a more reliable controller, it has been widely implemented to achieve good control performance and robustness. Most MPC algorithms are based on a linear model of a process and therefore the disadvantage associated with the linear controller is that it does not perform well over the wide range of operating conditions and with large disturbances [14]. As a result, a number of nonlinear model based control strategies have been developed recently [15–18].

Neural network modeling and neural network based model predictive control (NNMPC) are proposed and studied in this work for the modeling and control of a batch extractive distillation process, highly nonlinear behavior and complex process. Neural network forward and neural network inverse models are developed to predict the dynamics behavior and to control the process integrated with the dynamic optimization respectively. The obtained optimal neural network structure for the forward model has been employed to predict state variables over a predictive horizon incorporated into a MPC algorithm for searching optimal control actions via successive quadratic programming (SQP). To demonstrate the robustness of the NNMPC strategy, plant/model mismatches or uncertainties tests are performed and its control performance is compared with those of the NNDIC and PID approaches.

2. Process Description

Acetone and methanol have a normal boiling point of 56.14 $^{\circ}$C and 64.53 $^{\circ}$C, respectively. The mixture of acetone-methanol is an azeotrope property with a minimum boiling temperature of 55.24 $^{\circ}$C at atmospheric pressure. Then, the separation of the mixture by single batch or continuous distillation cannot be achieved. Therefore, a batch extractive distillation (BED) is proposed to handle this difficult task. The BED column is divided into two sections: a rectifying section and an extractive section as shown in Fig. 1.

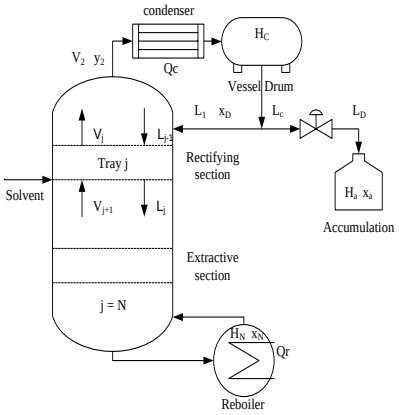


Fig. 1. Batch extractive distillation column.

The BED process operation can be carried out in 4 steps as follows:

1. Operation under total reflux without solvent feeding for steady-state operation (azeotropic composition).
2. Operation under total reflux with solvent feeding until maximum purity of acetone is reached.
3. Operation under finite reflux with solvent feeding to withdraw acetone until the desired purity of acetone is achieved.
4. Operation under finite reflux without solvent feeding to withdraw methanol until the desired purity of methanol is achieved.

A solvent feed of this process is water using for breaking of the acetone and methanol azeotropic composition. After operation in the 1st step is finished, the water is charged into the column. The acetone will be separated toward the top of the column while the methanol will be carried with water toward the column bottom in the 2nd and 3rd steps. In the rectifying section, due to the lack of methanol in this section, only the separation of acetone and water is performed. Pure acetone will preferably go to the top of the batch extractive distillation column. In the end of the 4th step, after the draw off of the acetone product in the main cut period and a slope cut period where the acetone in the column is completely depleted, the methanol product can be collected at the top of the column. The water can be collected at the bottom of the column. The distillate composition of acetone-methanol-water in the BED process is given in Fig. 2 [19].

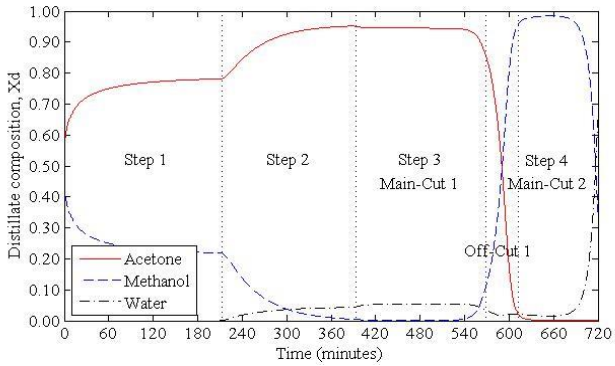


Fig. 2. Distillate composition of acetone-methanol-water.

The mathematical models of the BED process have been studied here. The meaning of letters and symbols are given in nomenclature. The column specifications, Antoine and NRTL parameters are summarized in Table 1, 2 and 3, respectively. To develop the mathematical models of the BED, following assumptions are made:

1. Constant tray efficiency.
2. Neglect of vapor holdup.
3. Perfect mixing on all trays and in all vessels.
4. Total condensation.

5. Ideal vapor phase for all components in mixture.
6. Heat duty constant.
7. Molar holdup constant.

Mathematical models of accumulator and condenser:

$$\frac{dH_a}{dt} = L_D \tag{1}$$

$$\frac{dH_a x_a}{dt} = L_D x_{Di} \tag{2}$$

$$\frac{dH_c x_{Di}}{dt} = V_2 y_{2i} - L_c x_{Di} \tag{3}$$

$$\frac{dH_c h_1^L}{dt} = V_2 h_2^V - L_c h_1^L - Q_c \tag{4}$$

Mathematical models of internal trays:

$$\frac{dH_j}{dt} = L_{j-1} + V_{j+1} - L_j - V_j \tag{5}$$

$$\frac{dH_j x_{ji}}{dt} = L_{j-1} x_{j-1,i} + V_{j+1} y_{j+1,i} - L_j x_{ji} - V_j y_{ji} \tag{6}$$

$$\frac{dH_j h_{ji}}{dt} = L_{j-1} h_{j-1}^L + V_{j+1} h_{j+1}^V - L_j h_j^L - V_j h_j^V \tag{7}$$

Mathematical models of the solvent feed tray:

$$\frac{dH_j}{dt} = L_{j-1} + V_{j+1} - L_j - V_j + F \tag{8}$$

$$\frac{dH_j x_{ji}}{dt} = L_{j-1} x_{j-1,i} + V_{j+1} y_{j+1,i} - L_j x_{ji} - V_j y_{ji} + F x_F \tag{9}$$

$$\frac{dH_j h_{ji}}{dt} = L_{j-1} h_{j-1}^L + V_{j+1} h_{j+1}^V - L_j h_j^L - V_j h_j^V + F h_F^L \tag{10}$$

Mathematical models of the reboiler:

$$\frac{dH_N}{dt} = L_{N-1} - V_N \tag{11}$$

$$\frac{dH_N x_{Ni}}{dt} = L_{N-1} x_{N-1,i} - V_N y_{Ni} \tag{12}$$

$$\frac{d(H_N h_N^L)}{dt} = L_{N-1} h_{N-1}^L - V_N h_N^V + Q_r \tag{13}$$

where $y_{j,i} = \gamma_{j,i} \frac{p_{s,j,i}}{p} x_{j,i}$ and $p_{s,j,i}(T)$ of the pure components are calculated by the Antoine equation as:

$$\log p_{s,j,i} = A - \frac{B}{T + C(^\circ C)} \tag{14}$$

For thermodynamic equations, the NRTL equation is used to find the liquid activity coefficient in the vapor liquid equilibrium calculated based on information given in Table 3 [20].

By NRTL equation:

$$\ln \gamma_i = \frac{\sum_{j=1}^{C} x_j \tau_{ji} G_{ji}}{\sum_{k=1}^{C} x_k G_{ki}} + \sum_{j=1}^{C} \frac{x_j G_{ij}}{\sum_{k=1}^{C} x_k G_{kj}} \left[\tau_{ij} - \frac{\sum_{k=1}^{C} x_k \tau_{kj} G_{kj}}{\sum_{k=1}^{C} x_k G_{kj}} \right] \tag{15}$$

where $G_{ij} = \exp(\alpha_{ij} \tau_{ij})$, $\tau_{ij} = a_{ij} + (b_{ij} / T)$, $\alpha_{ij} = c_{ij}$, $\tau_{ii} = 0$, $G_{ii} = 1$.

The calculated azeotropic composition of acetone and azeotropic temperature at atmospheric pressure from the NRTL equation are 77.75 mol% and 55.22 °C respectively which are in the range of 74.94- 81.60 mol% and 55.10-56.90 °C defined by the azeotropic compositions of acetone and azeotropic temperature on the top tray [20]. Therefore, the NRTL equation gives reliable liquid activity coefficients.

Six T-type thermocouple sensors are placed in various section of the column to continuously provide the measurement of the temperatures of the column and gas-liquid chromatography (type Varian 6000, Vista) has been used to analyze the composition of samples taken [21].

Table 1. Column specifications.

Parameters	Data
No. of ideal stages (including reboiler and condenser)	20
Reboiler maximum capacity (kmol)	52
Solvent feed flow rate (kmol/hr)	7
Feed composition (mol fraction, *x*)	
- Acetone	0.5
- Methanol	0.5
- Water	0.0
Column holdup (kmol)	
- Condenser (H_c)	0.1
- Internal plates (H_j)	0.5
Column pressure (bar)	1.013
Reboiler heat duty Q_r (MJ/hr)	4E+2

Table 2. Antoine parameters of the acetone-methanol-water system.

Components	A	B	C
Acetone (A)	7.02447	1.16000×10^3	2.2400×10^2
Methanol (B)	7.87886	1.47311×10^3	2.2300×10^2
Water (E)	7.96681	1.66821×10^3	2.2800×10^2

Table 3. NRTL parameters of the acetone-methanol-water system.

Component, *i*	Acetone	Acetone	Methanol
Component, *j*	Methanol	Water	Water
a_{ij}	0	6.3981	-0.6930
a_{ji}	0	0.0544	2.7322
b_{ij}	101.8859	-1808.9900	172.9871
b_{ji}	114.1347	419.9700	-617.2690
c_{ij}	0.3	0.3	0.3

3. Dynamic Optimization

In this work, the objective function of dynamic optimization is to maximize the weight of the distillate product of the 3rd step of the batch extractive distillation operation subject to a given product purity constraint. The internal reflux ratio is selected as the decision variable with fixed batch time and reboiler heat duty.

Mathematically, the problem can be formulated as:

$$\underset{R(t)}{Max} \quad H_a \tag{16}$$

Subject to

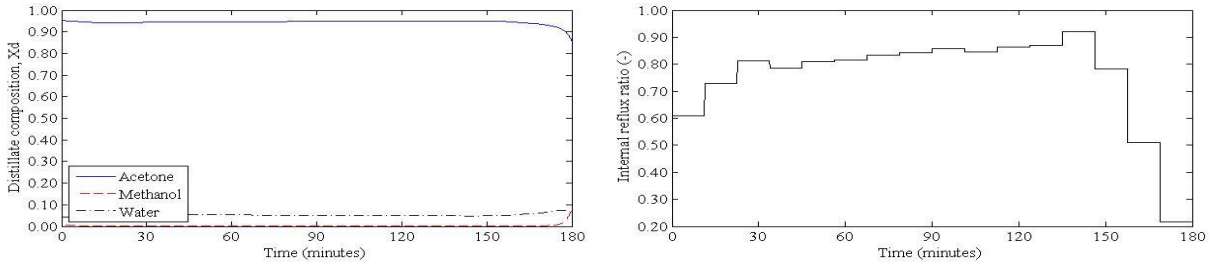
$$f(t, \dot{x}, x, u, v) = 0 \tag{17}$$

$$x_{a,1} \geq 0.94 \tag{18}$$

$$0 \leq R \leq 1 \tag{19}$$

$$t_f = 3 \tag{20}$$

A dynamic optimization problem for the BED is transformed into a nonlinear programming (NLP) problem solved by a SQP-based optimization technique and the process models are integrated by the Gear's type method. The maximum weight of the distillate product with respect to various time intervals: 2, 4, 8 and 16 intervals are determined. The simulation results with 16 intervals are shown in Fig. 3. Table 4 reports the distillate composition in the accumulator and the amount of the desired product of each time interval. It can be seen that the dynamic optimization strategy with two or more time intervals can drive the purity of the distillate product to the given high purity specification. In addition, the increase in time intervals can produce more distillate product. However, the maximum product of 511.25 kilogram of acetone is achieved in the case of 16 time intervals. The simulation results show that the internal reflux ratio is gradually increased to achieve the product in the accumulator ($x_{a,1}$ = 0.94) as defined, and then is decreased during the product is withdrawn as shown in Fig. 3(b). The obtained acetone distillate composition profile (as shown in Fig. 3(a)) is then used as the set point of each controller studied to achieve maximum weight of acetone with specified purity.



(a) (b)

Fig. 3. Optimal operation profile of 16 time intervals (a) Distillate composition (b) Internal reflux ratio.

Table 4. Summary of the optimal results in a nominal case.

Intervals	$X_{a,1}$ (t_f)	H_a (kg)
1	0.94	477.4812
2	0.94	479.6315
4	0.94	493.8426
8	0.94	508.2045
16	0.94	511.2520

4. Neural Network based Modeling

In this part, neural networks modeling have been applied to give prediction of the distillate mole fraction profiles of acetone, methanol, water and the temperature profile on the top tray of column in the BED process. The feedforward topology and supervised learning algorithm via the Levenberg-Marquardt method have been used to determine the structure of the neural network model. An algorithm for obtaining the neural network model has been reported by Daosud [6]. The neural network forward model is trained with possible scenarios consisting of parametric certainty and uncertainties of the plant (nominal case, -5%γ_1 and +10%γ_3). To ensure good closed-loop performance, the sampling interval should be small to adequately capture the dynamics of the process. In this work, the process data gathered are considered only after the total reflux operation is ended – that means the distillate can be withdrawn to the accumulator (3rd step). In each scenarios, a step change in the manipulated variable (reflux ratio) is introduced and obtained process data are sampled every 1 minute. Process data from each pattern are gathered and randomly divided into 3 sets: 60 percentages of total data for training, 30 percentages of total data for testing, and 10 percentages of total data for validating. The input data in input layers for neural network training has ten inputs. It consists of the past and the present values of the distillate mole fraction of acetone ($x_{d,1}$(k-1), $x_{d,1}$(k)), the distillate mole fraction of methanol ($x_{d,2}$(k-1), $x_{d,2}$(k)), the distillate mole fraction of water ($x_{d,3}$(k-1), $x_{d,3}$(k)), the top tray temperatures (T_2(k-2), T_2(k-1), T_2(k)) and the internal reflux ratio (R(k)) at present time interval which is the manipulated variable of the BED process respectively. The output data in the output layers consists

of the predicted values in the future (k+1) of distillate mole fraction of acetone, methanol, water and temperature on the top tray of column as shown in Fig. 4.

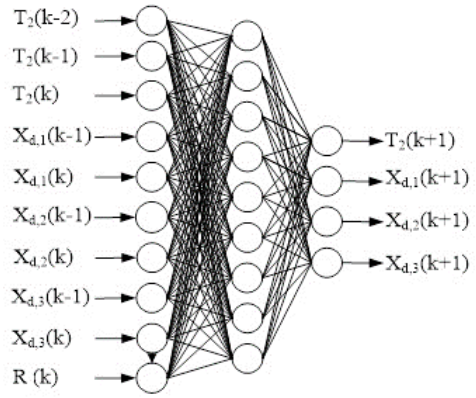


Fig. 4. Architecture of neural network forward model.

Mean square error (MSE) [15] given in Eq. (16) is used to examine the accuracy of training output with validated data sets and examine the number of nodes to achieve an optimal architecture.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - p_i)^2 \tag{21}$$

where y_i is the training output, p_i is target value or validated data sets and N is number of data sets.

An optimal architecture of the neural network forward model can be achieved by the minimization of the MSE with respect to the variation of the hidden node between 1 and 20 nodes. The MSE error is then monitored and the one that corresponds to the minimum MSE value is selected for determining the number of the hidden node. The simulation shows that the optimal architecture of the neural network forward model with sigmoid transfer functions in the hidden layer and linear transfer functions in the output layer is [10-16-4] (10 nodes in input layer, 16 nodes in hidden layer and 4 nodes in output layer). The MSE index for the test with the validating data of this architecture is 1.80×10^{-9}. Then, the obtained optimal neural network is applied to predict the dynamic behavior of the system in MPC algorithm.

5. Neural Network Direct Inverse Control

A neural network inverse model is applied to formulate a neural network direct inverse controller (NNDIC) to control the process. The architecture of the neural network inverse model is similar to that of the neural network forward model whereas the prediction of output is replaced by the control input. The neural network inverse model is used in NNDIC strategy to predict reflux ratio (R) which is the manipulated variable of this process.

The model consists of eleven nodes in the input layer and one node in the output layer. The network inputs consists of the acetone distillate composition ($x_{d,1}$) at time k-1 , k and k+1, the methanol distillate composition ($x_{d,2}$) and the water distillate composition ($x_{d,3}$) at time k-1 and k, the top tray temperatures (T_2) at time k-1 and k and the internal reflux ratio (R) at time k-1 while the network output is the predicted values of the reflux ratio at time k. The MSE minimization is investigated to find the optimal architecture of neural network inverse model. The simulation shows that the optimal architecture of neural network inverse model is [11-12-1] with the MSE index of 2.10×10^{-9} for the test with validating data. Then, the obtained optimal neural network inverse model is utilized in the NNDIC strategy for tracking the acetone distillate composition. The NNDIC strategy for controlling the acetone distillate composition is illustrated as Fig. 5.

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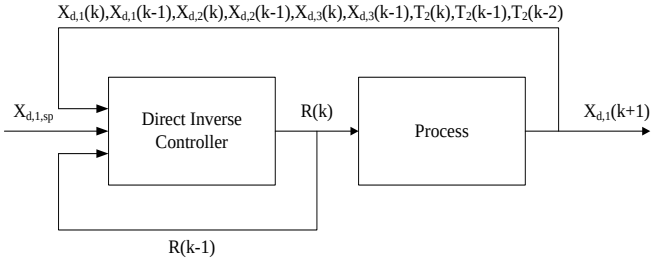


Fig. 5. Flow diagram of the proposed NNDIC strategy.

6. Neural Network based Model Predictive Control (NNMPC)

The concept of MPC is to determine a profile of control actions for a time horizon minimizing an objective function subject to a dynamic process model and system constraints. At each control interval, a set of manipulated variables is computed in such a way to optimize the future behavior of the process, but only the first element of control set is applied. Then, the optimization procedure, based on new information, is repeated to modify a new control set with the control and prediction horizons moving forward one sampling time step.

Here, the neural network forward model, [10-16-4] architecture as obtaining from the previous section is used to determine future outputs over the prediction horizon (*P*). After that, the predicted outputs are incorporated into an optimization routine to calculate the internal reflux ratio (control action) profile according to a minimal sum of squares of the errors between the predicted outputs and the set point values and the control moves evaluated over the prediction horizon via a successive quadratic programming (SQP) algorithm. The NNMPC formulation can be written as follows:

$$\min_{R(k),\ldots,R(k+m-1)} \sum_{i=1}^{P} [W_1\{x_{a,1,sp}(k+i) - \hat{x}_{a,1}(k+i)\}^2 + W_2\{\Delta R\}^2] \tag{22}$$

Subject to

$$0 < R < 1.0 \tag{23}$$

$$0 < x_{d,1} < 1.0 \tag{24}$$

$$x_{d,1}(k+P) = x_{d,1,sp}(k+P) \tag{25}$$

Figure 6 shows the data flow diagram of the NNMPC. At the first prediction, an initial reflux ratio at time k is introduced into the model. With the NN models of the BED, the output at time k+1 is determined and then used as an input in the second prediction. After M steps prediction, the reflux ratio is kept constant and equal to the reflux ratio at time k+*M*+1. Various trials have been carried out through simulations to find the set of control parameters (Internal reflux ratio profile). The tuning parameters: the prediction horizon (*P*), the control horizon (*M*), the weight of control variable (W_1) and the weight of manipulate variable (W_2) are chosen as three, three, ten and ten respectively.

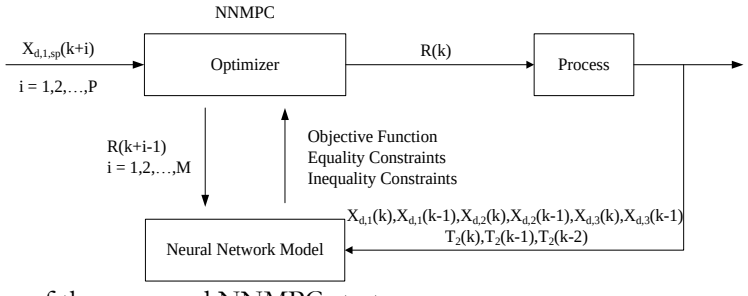


Fig. 6. Flow diagram of the proposed NNMPC strategy.

7. Simulation Result

The purpose of this simulation study is to evaluate the control performance of the NNMPC compared to those of the NNDIC and PID approaches. The NNMPC has been applied to provide the tracking of the acetone distillate composition profile by adjusting the internal reflux ratio. In the presence of plant

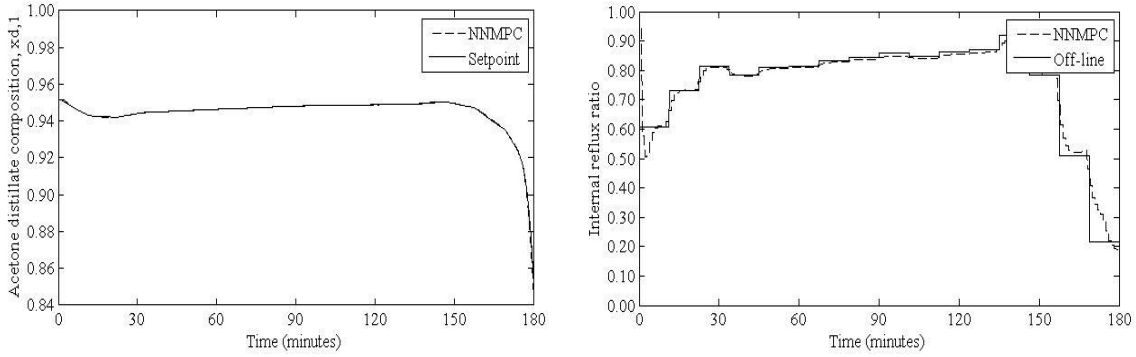
uncertainties (5% decreasing of γ_1 and 10% increasing of γ_3 from their nominal values), the NNMPC, NNDIC and PID controllers are tested without any changes in the tuning parameters. Each controller is introduced after the total reflux operation is ended. The closed loop performances of the NNMPC, NNDIC and PID are indicated by the integral of absolute value of the error (IAE), the acetone distillate product purity at the end of operation, $x_{d,1}(t_f)$, and the weight of distillate product (H_a).

For the set point tracking case, each controller is applied to track the acetone distillate composition at the desired profile. Figures 7, 8 and 9 show the acetone distillate composition using NNMPC, NNDIC and PID respectively. The results indicate that NNMPC gives very good distillate composition tracking and smooth control movement (reflux ratio) as shown in Figs. 7(a) and 7(b), respectively. This is because the distillate composition is an equality constraint in the optimization algorithm and the neural network model used in the NNMPC is trained covering the possible parametric plant uncertainties as described in the section 4. The movement of the reflux ratio is smooth because minimum control moves are incorporated in the objective function of the NNMPC algorithm. For the PID, the results show that it can give good distillate composition tracking with a bit oscillated control movement as illustrated in Figs. 8(a) and 8(b) respectively. For the NNDIC, the results show that it provides oscillated response of the controlled variable around the desired profile as shown in Fig. 9(a) and the reflux ratio changes drastically as shown in Fig. 9(b). The performance indices of all control strategies are summarized in Table 5.

Table 5. Close-loop performance of NNMPC, NNDIC and PID control.

Controller	IAE	$X_{a,1}$	H_a (kg)
1) Nominal Case			
NNMPC	0.9810	0.9403	509.0228
NNDIC	0.9827	0.9403	508.0603
PID	0.9806	0.9403	509.8167
2) -5%γ_1			
NNMPC	0.0751	0.9400	207.2936
NNDIC	0.1400	0.9400	206.6708
PID	0.1046	0.9400	206.8086
3) +10%γ_3			
NNMPC	0.1270	0.9400	141.0023
NNDIC	0.1317	0.9400	140.8705
PID	0.0789	0.9400	141.1105

† IAE = the integral of absolute value of the error



(a) (b)

Fig. 7. Set point tracking with NNMPC (nominal case) (a) Acetone distillate composition (b) Reflux ratio.

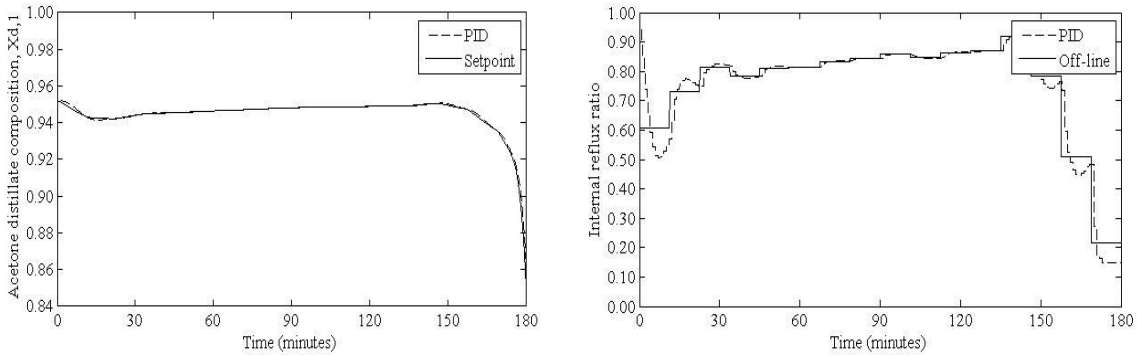


Fig. 8. Set point tracking with PID (nominal case) (a) Acetone distillate composition (b) Reflux ratio.

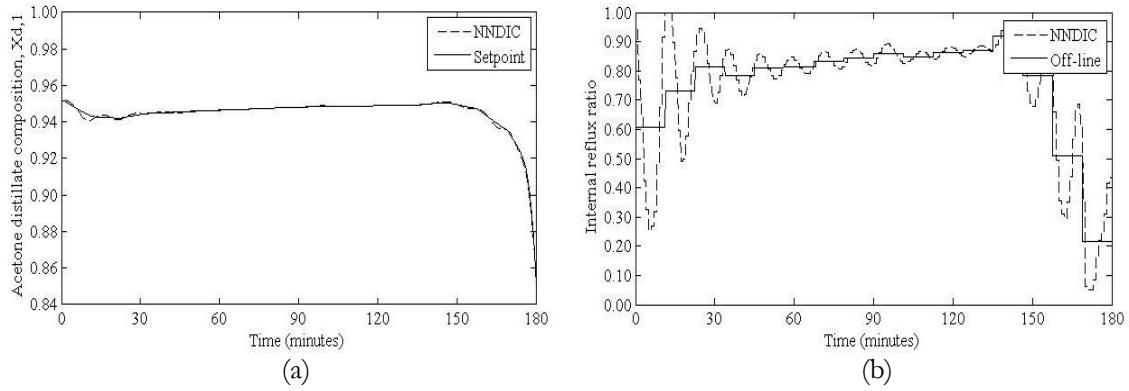


Fig. 9. Set point tracking with NNDIC (nominal case) (a) Acetone distillate composition (b) Reflux ratio.

In the presence of plant uncertainties, the vapor-liquid equilibrium constants are changed by decrease in γ_1 of 5% and increase in γ_3 of 10% from their nominal values. Figure 10 shows the acetone distillate composition using NNMPC in the case of the decrease in γ_1 of 5%. The results show that the NNMPC can give reasonably good distillate composition control in this case. Additionally, the control move (reflux ratio) is still smooth as good as in the nominal case. While the NNDIC can give reasonably good distillate composition control but the reflux ratio movement is drastic at the beginning and gradually depleted until achieving the desired purity product. Similarly, the PID can provide reasonably good distillation composition control, but the control performance is the worst.

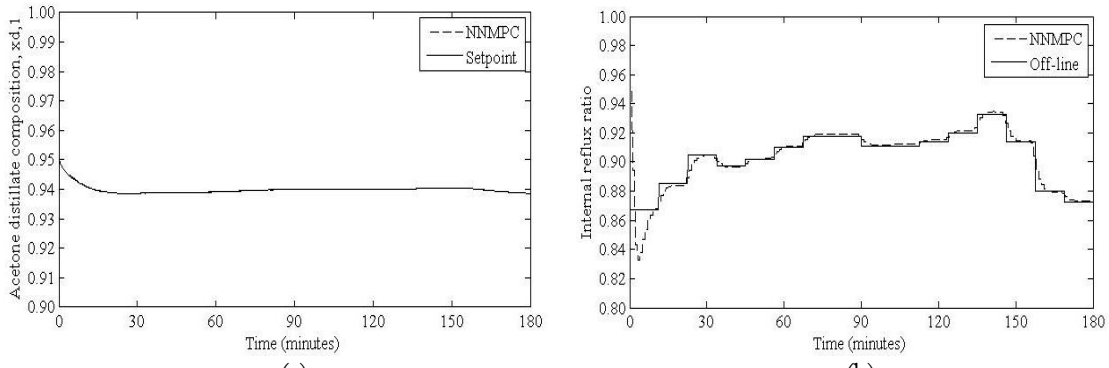


Fig. 10. Set point tracking with NNMPC (-5%γ_1) (a) Acetone distillate composition (b) Reflux ratio.

The control performance indicators (IAE, distillate composition and the weight of acetone) of each controller are summarized in Table 5. It was found that the NNMPC provides the best control performance among the NNDIC and the conventional PID in all cases. All controllers can maintain the

distillate product purity on its specification in the all cases. The distillate amounts obtained from the NNMPC and NNDIC are a little bit lower than that obtained from the optimal policy presented in the section 3. The NNMPC control moves are smooth in all cases. Although the NNDIC can keep the final distillate product on its specification, the control moves (reflux ratio) are very drastic. This shows the applicable of the NNMPC in the real plant over the NNDIC and PID.

8. Conclusion

The neural network based model predictive control has been studied and investigated to control a batch extractive distillation column used for the separation of waste solvent mixture of acetone and methanol. A predefined (off-line) set point is determined by a dynamic optimization strategy. The objective function of dynamic optimization strategy is to maximize the weight of a distillate product subject to a given acetone specification (94.0% by mole of acetone), constant reboiler heat duty and batch operating time. Then, neural network model predictive control (NNMPC) is formulated to provide tracking of the predefined optimal set point. The robustness of the proposed controller has been tested with respect to parametric plant uncertainty: vapor-liquid equilibrium constants. It has been found that although each controller can keep the distillate product purity on its specification, the NNMPC gives the best control performance among the NNDIC and PID controller; the NNMPC provides the smoothest controller action without any drastic change.

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Nomenclature

h_i^L Liquid enthalpy at stage j (kJ/kmol)
h_i^V Vapor enthalpy at stage j (kJ/kmol)
h_F^L Liquid enthalpy of entrainer (kJ/kmol)
H_j Molar holdup at stage j (kmol)
L_j Molar liquid flow rate at stage j (kmol/hr)
V_j Molar vapor flow rate at stage j (kmol/hr)
Q_c Condenser duty (kJ/hr)
Q_r Reboiler duty (kJ/hr)
R Internal reflux ratio
T Temperature (K)
p Pressure (bar)
F Entrainer feed flow rate (kmol/hr)
x Liquid composition
y Vapor composition
W Weighting factor
γ Liquid-phase activity coefficient
$x_{d,i}$ Distillate liquid of component i
$x_{a,i}$ Accumulate liquid of component i
L_c Molar liquid flow rate on condenser
$x_{j,i}$ Liquid mole fraction of component i at stage j

$y_{j,i}$ Vapor mole fraction of component i at stage j
x_F Liquid mole fraction of entrainer
H_a Molar holdup at accumulator (kg)
t_f Final time (hr)
n_c Number of components

Subscripts:
i Component number
j Stage number
a Accumulator
c Condenser
r Reboiler
d Distillate

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