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Control of methylamine removal reactor using neural network based model predictive control

Liu Zhi Long, Yang Feng, Zhou Ke Jun, Xu Mei

Abstract—**Methylamine (MA) removal process using mixed bacteria strains depends highly on constant temperature (303 K), at which the mixed bacteria strains provide highest activity in removing MA. Controlling MA removal reactor is extremely difficult for its inherent process nonlinearities and complex reaction kinetics and other uncertain factors. In the designed approach, a network predicted model is trained as a nonlinear process to predict the future output of the controlled process according to current and previous input and output over the specified horizon. The advanced predictive control strategy is used to minimize the cost function in order to calculate the optimal output of the controller. In this work, a neural network based predictive control (NNMPC) algorithm was implemented to control the temperature of MA removal reactor and the controller performance in set-point tracking and disturbance rejection was investigated, and the performance results of NNMPC was compared with conventional PID controller. It is concluded that the NNMPC performance is superior to the conventional PID controller in the control of MA removal reactor.**

I. Introduction

METHYLAMINE (MA), a kind of important aliphatic amine, is one of the basic organic chemical raw materials. It is mainly used in the production of pesticides, corrosion inhibitors, medicine, fuel, emulsifiers and rubber production [1]. MA is present in organic industrial wastewater, such as the fermentation broths used for ethanol production [2]. The wastewater containing methylamine can cause serious water pollution, such as water eutrophication, and even threaten the health of human [3]. Therefore, it is significant to remove MA from wastewater [4]. However, methylamine removal reactor involves complex reaction mechanisms and the removal process is highly nonlinear in nature. The control of methylamine removal reactor is difficult due to its inherent process nonlinearities and complex reaction kinetics, and few researches have been conducted to research the advanced control strategies for methylamine removal reactor in recent years.

Model predictive control (MPC), an advanced process control technology, is widely implemented in industrial applications recently [5, 6]. MPC improves the control performance in terms of accuracy and robustness since the application of strategies of multi-step prediction, rolling optimization and feedback correction. The MPC algorithm uses an explicit process model to predict the future behavior of the plant and most of the MPC strategies are based on linear models of the process which offers poorer performance in controlling the methylamine removal reactor for its inherent process nonlinearities and complex reaction kinetics [7].To overcome the difficulties connected with nonlinear factors and complex reaction kinetics of methylamine removal reactor, an MPC based on a nonlinear model is desirable [8]. Recently, neural network plays an important role in the identification and construction of models with complex nonlinear factors, and then neural network can offer an alternative nonlinear modeling approach for MPC [9-11].The combination of neural network and MPC approach can overcome the shortcoming of traditional linear MPC which cannot effectively control the model with highly nonlinear factors [12-13]. Neural network acts as a feed-forward process model predicting the output of the nonlinear process in the neural network model based prediction control [14].

In this work, a neural network model based prediction controller (NNMPC) was developed for the control of methylamine removal reactor experimentally, and this kind of experiments haven't been conducted in recent years. The model of methylamine removal reactor was constructed using a neural network with one hidden layer with 9 neurons and then the MPC strategy was used to calculate the optimal control inputs to control the process so that the temperature of the methylamine removal reactor was assured. Conventional PID controller was also used in the experiment and the performance of used controllers were compared and analyzed.

II. Methylamine Removal Reactor Modeling

A schematic diagram of the experimental methylamine removal reactor is shown in Fig. 1. In order to obtain maximum efficiency of methylamine removal process, the temperature of the reactor must be kept at 303 K, at which the mixed bacteria strains have highest activity in removing MA. So, the controlled variable is the temperature of the experimental methylamine removal process. The flow rate of the coolant is selected as the control variable among the input variables, whereas the other variables keep constant. Considering the methylamine removal process using mixed

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bacteria strains is exothermic, the circulating water bath can keep the process at a constant temperature by adjusting the flow rate of the coolant. The methylamine removal reactor uses a 100 L jacketed glass reactor. Thermocouple is used to measure the real-time temperature of the reaction process since the efficiency of methylamine removal process is highly dependent on temperature. The mixture inside the reactor is stirred using a turbine agitator, the speed of which can adjust in the range of 50–2000 rpm. In this study, speed of stirring turbine agitator is 800 rpm.

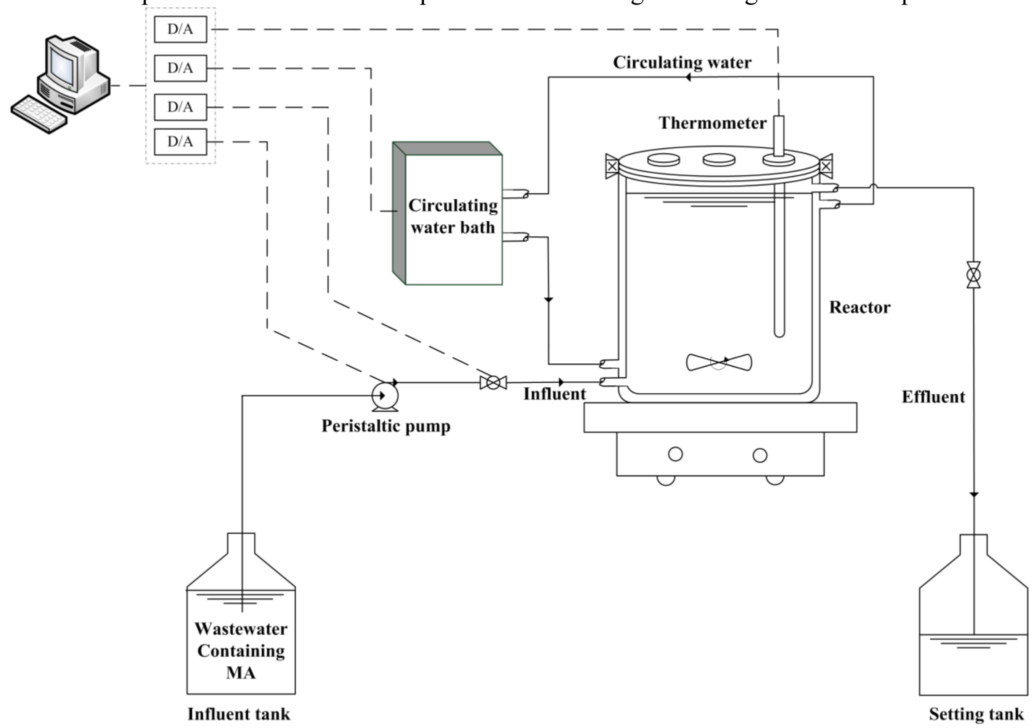

Fig.1. Experimental setup for the methylamine removal.

The mathematical model of the methylamine removal reactor is derived under several simplifying assumptions. The density of the wastewaterρ_l, the density of coolantρ_c, the specific heat capacity of wastewater C_p and the specific heat capacity of coolant C_{pc} re assured to be constant. The simplified non-linear dynamic mathematical model of the methylamine removal reactor is described by two partial differential equations

$$\frac{dC_A}{dt} = \frac{q}{v}(C_{A0} - C_A) - k_0 C_A e^{-\frac{E}{RT}} \tag{1}$$

$$\frac{dT}{dt} = \frac{q}{v}(T_f - T) + k_1 C_A e^{-\frac{E}{RT}} + k_3 q_c (1 - e^{-\frac{k_2}{q_c}})(T_c - T) \tag{2}$$

Where, C_{A0} -Concentration of wastewater with MA, C_A-Concentration of wastewater without MA, q-Flow rate of wastewater with MA, q_c-Flow rate of coolant, v-Volume of methylamine removal reactor, T_f -Temperature of wastewater with MA, T -Temperature of methylamine removal process,T_c-Temperature of coolant,E/R-Activation energy, time constant k_1, k_2, k_3 are calculated as follows

$$k_1 = -\frac{\Delta H k_0}{\rho_1 C_p} \tag{3}$$

$$k_2 = \frac{h_a}{\rho_1 C_{pc}} \tag{4}$$

$$k_3 = -\frac{\rho_c C_p}{\rho_1 C_p v} \tag{5}$$

Here, ΔH -Heat of reaction, k_0 -Exponential factor, h_a-Heat-transfer coefficient, ρ_1- Density of wastewater with MA, ρ_c- Density of coolant. Parameters and steady-state inputs of the methylamine removal reactor are enumerated in TABLE I.

The steady-state analysis of the MA removal reactor was shown in Fig.2, which demonstrated the dependence of temperature of the MA removal process on the flow rate of coolant. It confirmed that the MA removal reactor contains highly nonlinear factors.

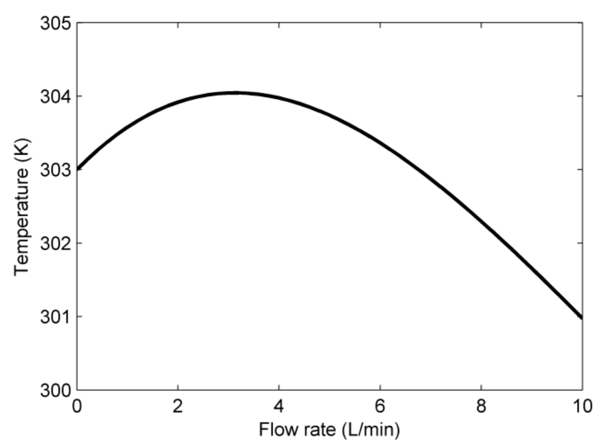

Fig.2. Steady-state analysis of the MA removal reactor.

TABLE I
MA REMOVAL REACTOR PARAMETERS AND STEADY-STATE INPUTS

Variable	Value	Unit
C_{A0}	0.50	*mol/L*
C_A	0.48	*mol/L*
T_f	310.00	*K*
T_c	285.00	*K*
T	303.15	*K*
q	10.00	*L/min*
q_c	3.80	*L/min*
v	100.00	*L*
ρ_l	1×10^3	*g/L*
ρ_c	1×10^3	*g/L*
C_p	1.00	*cal/g·K*
C_{pc}	1.00	*cal/g·K*
h_a	7.20×10^5	*J/min·K*
k_0	7.20×10^{10}	*min^{-1}*
ΔH	-2.00×10^5	*cal/mol*

III. NEURAL NETWORK BASED MODEL PREDICTIVE CONTROL

Several researches have confirmed the successful application of data-based modeling methods such as neural network in the field of industry processes [15-19]. In recent years, some process systems have witnessed the extensively application of artificial intelligence approaches using artificial neural networks [15], [20-22].The recent upsurge of researching neural network has promoted the application for identifying nonlinear system which even contains noise and uncertain factors using neural network [23-25].

It is important for MPC to getting the predictive model of the controlled plant, which can predict the output of the system using the current input and output value. In nature, MPC use a kind of optimization algorithm which can optimizes the objective function subject to the model of plant and some constraint functions over a finite time horizon. Fig. 3 shows the schematic diagram using neural network identifier as a predictive model.

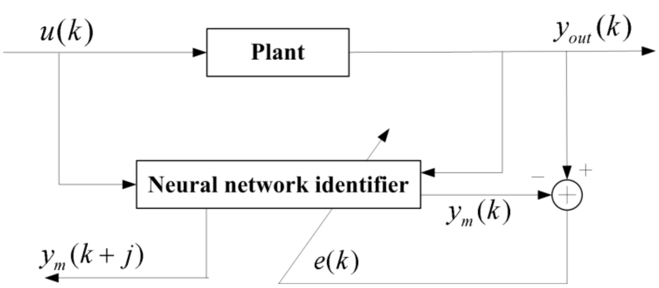

Fig.3. Schematic diagram using neural network identifier as predictive model.

The neural network identifier predicts the future output of the plant $y_m(k+j), (j=1,2,\cdots,P)$, according to the input u and output y_{out} of the controlled system. The vector form of $y_m(k+j)$ is expressed as follows

$$Y_m(k+1)=[y_m(k+1),\ \ y_m(k+2),\cdots,y_m(k+P)]^T \tag{6}$$

where, P is the predictive time horizon.

Considering the effects caused by model identify error, external disturbances and other uncertain factors, the output error of predictive model and actual controlled model in current time $e(k)=(y_{out}(k)-y_m(k))$ is calculated as a feedback correction in order to obtain the corrected predicted output in future time, which is determined as

$$y_p(k+j)=y_m(k+j)+h_j e(k), j=1,2,\cdots,P \tag{7}$$

where, h_j is the feedback correction coefficient.

In order to provide the smooth running and good dynamic characteristics of the system, the output of the system is demanded to reaches the set value along a pre-specified reference trajectory. The control strategy of multi-step prediction model is shown in Fig. 4.

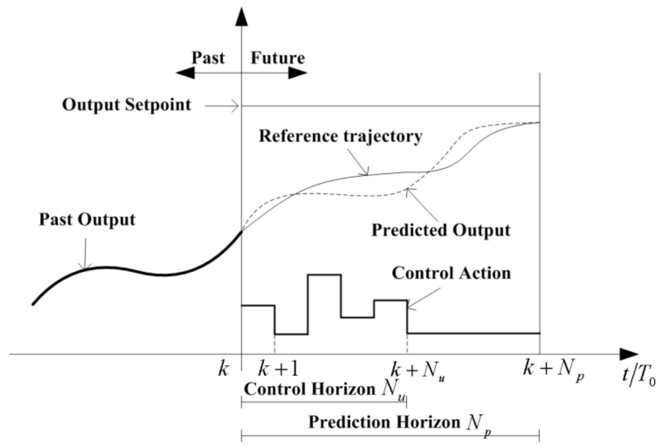

Fig.4. Control strategy of multi-step prediction model.

Generally, the reference trajectory $y_r(k)$ is an exponential curve leaving from the current actual output of the system $y_{out}(k)$, which is expressed as follows

$$y_r(k+i)=\alpha_r y_{out}(k)+(1-\alpha_r)y_s(k), i=1,2,\cdots \tag{8}$$

where, α_r is the parameters of reference trajectory; $y_s(k)$ is the set value.

With reference trajectory and predicted output, the performance of rolling optimization can be established to calculate the control signal. The performance objective function is determined as

$$J=\sum_{j=1}^{N_p}\theta_j[y_r(k+i)-y_p(k+i)]^2+\sum_{i=1}^{N_u}\lambda_i[u(k+i-1)]^2 \tag{9}$$

where, N_p is prediction horizon and N_u is control horizon, θ_j and λ_i are the weighting factors of tracking error and control signal. In order to calculate the control rate conveniently, the objective function can be expressed as

$$J=(\mathbf{Y}_r(k+1)-\mathbf{Y}_\mathbf{p}(k+1))^T\boldsymbol{\theta}(\mathbf{Y}_r(k+1)-\mathbf{Y}_\mathbf{p}(k+1))+\mathbf{U}^T(k)\boldsymbol{\lambda}\mathbf{U}(k) \tag{10}$$

where, $\mathbf{Y}_r(k+1)=[y_r(k+1),y_r(k+2),\cdots,y_r(k+N_p)]^T$, $\mathbf{U}(k+1)=[u(k),u(k+1),\cdots,u(k+N_u-1)]^T$ and assuming that the control value will stay constant since the time $k+N_u-1$,which also means $u(k+N_u-1)=u(k+N_u)=\cdots=u(k+N_p-1)$. $\boldsymbol{\theta}$ and $\boldsymbol{\lambda}$ are the weighting factor matrix of tracking error and control signal, which are expressed by two diagonal matrixes

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_1 & & & \\ & \theta_2 & & \\ & & \ddots & \\ & & & \theta_{N_p} \end{bmatrix}, \quad \boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_{N_u} \end{bmatrix} \tag{11}$$

Ordering that $\partial J / \partial \mathbf{U}(k) = 0$, the optimized control output $\mathbf{U}(k)$ is determined as

$$\mathbf{U}(k) = (\mathbf{G}^{\mathbf{T}} \boldsymbol{\theta} \mathbf{G})^{-1} \mathbf{G}^{\mathbf{T}} \boldsymbol{\theta} (\mathbf{Y}_{\mathbf{r}}(k+1) - \mathbf{F}\mathbf{U}(k-1) - \mathbf{h}e(k)) \tag{12}$$

$$\mathbf{G} = \begin{bmatrix} g_1 & & & \\ g_2 & g_1 & & \\ \vdots & \vdots & \ddots & \\ g_{N_u} & g_{N_u - 1} & \cdots & g_1 \\ \vdots & \vdots & & \vdots \\ g_{N_p} & g_{N_p - 1} & \cdots & g_{N_p - N_u + 1} \end{bmatrix}_{N_p \times N_u} \tag{13}$$

$$\mathbf{F} = \begin{bmatrix} g_N & g_{N-1} & \cdots & g_{N-N_p+1} & \cdots & g_2 \\ & g_N & \cdots & g_{N-N_p+2} & \cdots & g_3 \\ & & \ddots & \vdots & & \vdots \\ & & & g_N & \cdots & g_{N_p+1} \end{bmatrix}_{N_p \times (N-1)} \tag{14}$$

where, $\mathbf{G}$ and $\mathbf{F}$ are coefficient matrixes, which are constituted by the coefficients of impulse responses. g_i is the impulse responses sequence of the controlled object, $g_i (i = 1, 2, \cdots, N)$, and N is the impulse response truncation length of the model.

The neural network model based prediction controller contains the neural network model which act as the controlled process to predict the future output of the process. With reference trajectory and predicted output the optimization algorithm is used to calculate the proper output of the controller. The structure of NNMPC is shown in Fig. 5.System identification that constructing the neural network model is the first step in designing NNMPC, in which a two-layer network with liner transfer functions in the output layer and sigmoid transfer functions in the hidden layer is used.

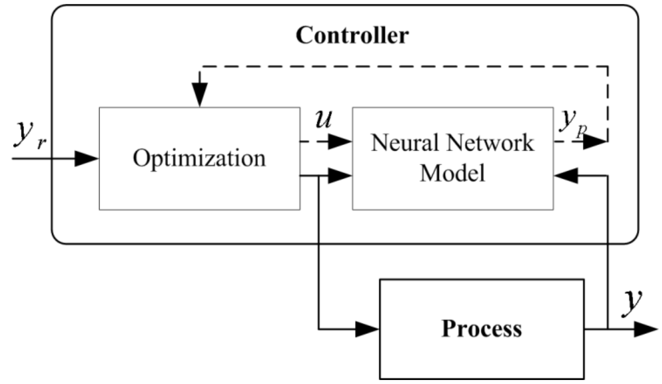

Fig.5. Neural network model based prediction controller.

During the neural network modeling process, the network is trained by the error between plant output and the neural network output. The neural network is used to predict the future plant output according to the previous input and output of the model in NNMPC. Fig. 6 shows the structure of the neural network model, where $y_p(k)$ is neural network output, $u(k)$is the plant input, $y(k)$ is the plant output, the TDL blocks are the tapped delay lines, $\mathbf{IW}^{i,j}$is the weight from the input number $\boldsymbol{j}$ to the layer number $\boldsymbol{i}$, $\mathbf{LW}^{i,j}$is the weight matrix from the layer number $\boldsymbol{j}$ to the layer number $\boldsymbol{i}$, $\mathbf{b}^1$ is bias of the hidden layer, b^2 is the bias of the output layer.

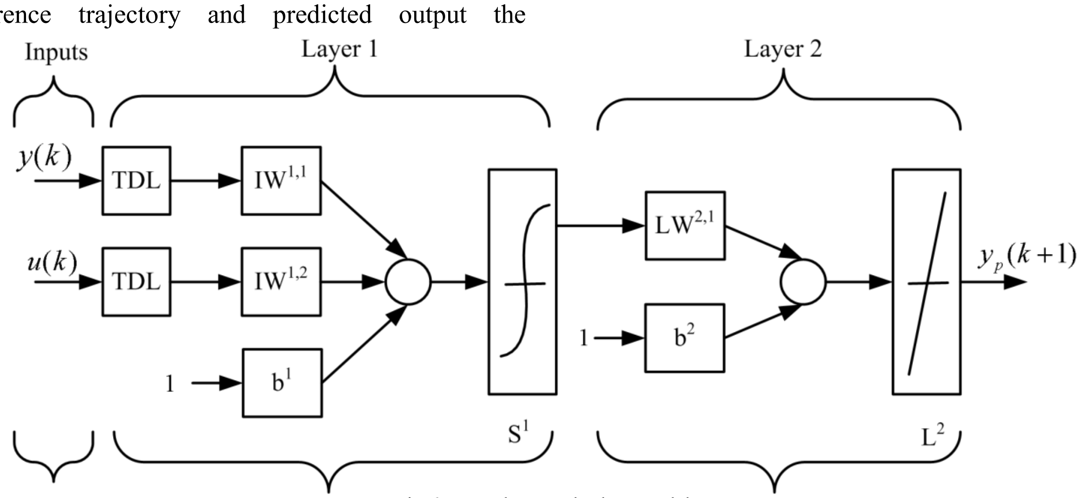

Fig.6. Neural network plant model.

IV. CONTROL OF METHYLAMINE REMOVAL REACTOR

The controlled process is the MA removal reactor described in Section 2, and the control algorithm is NNMPC described in Section 3. The training data were obtained from the nonlinear model of the MA removal reactor (1)-(5) and the network was trained offline. The parameters of neural network prediction model and the parameters of plant identification are shown in TABLE II. Fig.7 and Fig.8 show the training result obtained from training and validation data respectively. Considering that the identification error is sufficiently small in both case and the plant actual output and the neural network output fit well, the neural network training and model identification were successful.

Once the neural network prediction model was obtained, the control for the MA removal reactor was started, using NNMPC. The chosen parameters for prediction control of MA removal actor with NNMPC were shown in TABLE III.

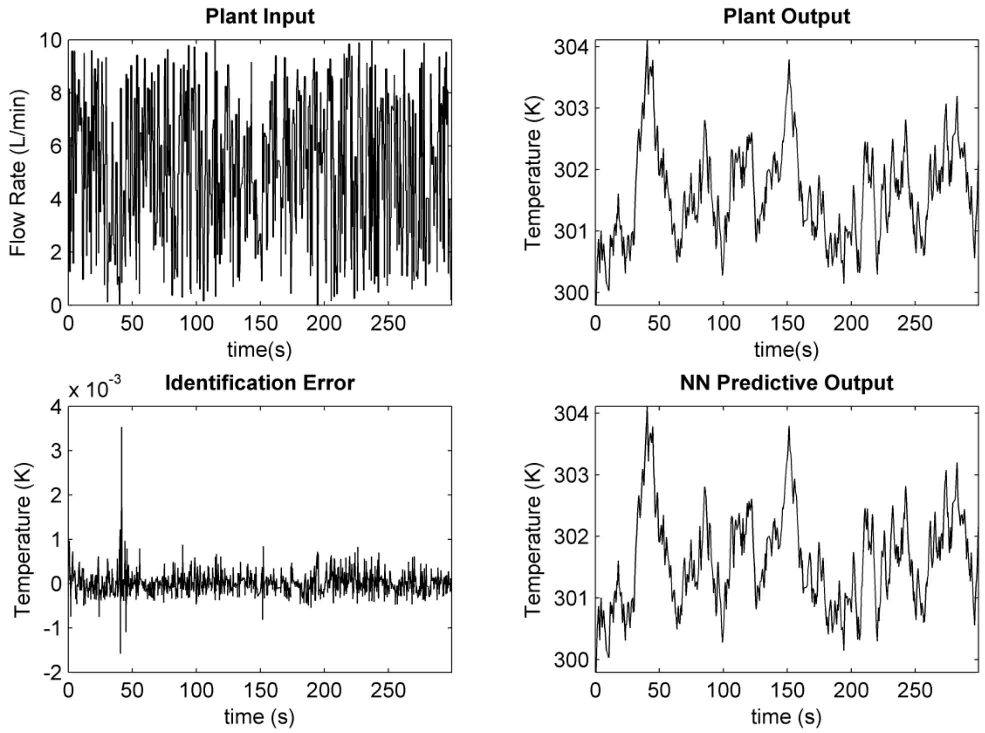

Fig.7. Training data for neural network model.

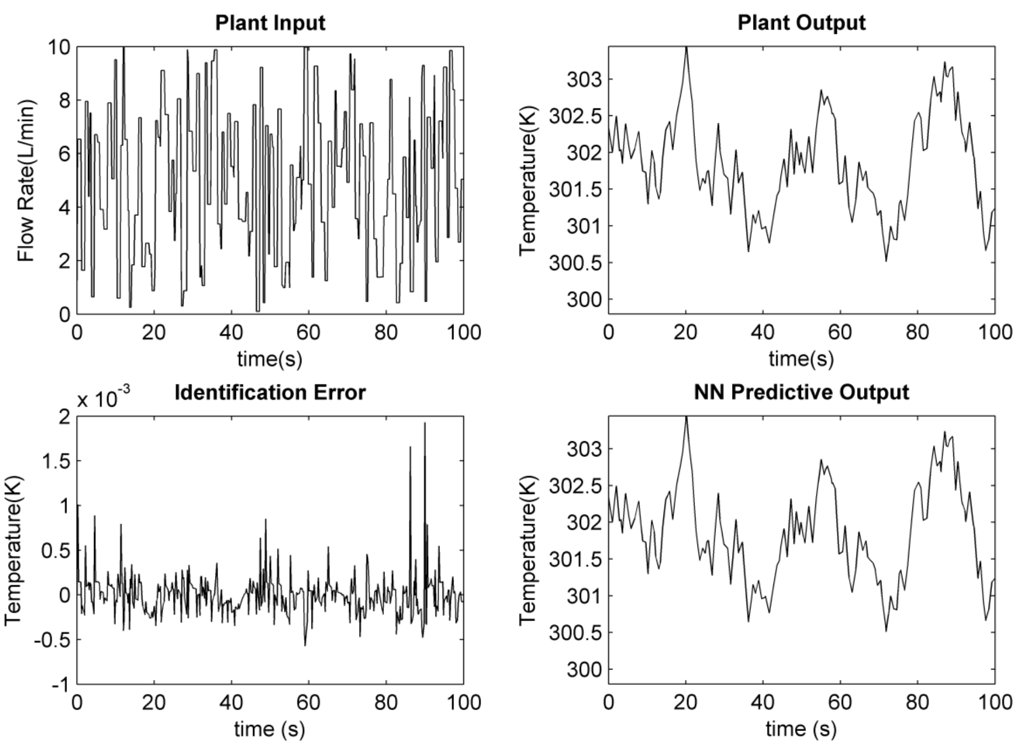

Fig.8. Validation data for neural network model.

TABLE II
PARAMETERS OF NEURAL NETWORK MODEL IDENTIFICATION

Parameters	Value
No. of input nodes	6
No. of hidden layer nodes	9
No. of delayed plant input	2
No. of delayed plant output	2
No. of output nodes	1
Maximum plant input	10 L/min
Minimum plant input	0 L/min
Maximum plant output	315 K
Minimum plant output	285 K
Total sample size	2,000
Training function	Levenberg-Marquardt method
Training epochs	400
No. of input nodes	6
No. of hidden layer nodes	9

TABLE III
PARAMETERS OF PREDICTION CONTROL OF MA REMOVAL ACTOR

Parameters	Value
Prediction horizon	27
Control horizon	15
Sampling interval	2 s
Control weight factor	0.05
Searching factor	0.001
Minimization routine	Backtracking optimization[26]

The control input constrains were 1 L/min<q_c<10 L/min and the control output constrains were 285 K<T<315k. The NNMPC block was implemented in MATLAB-Simulink.

V. RESULTS AND DISCUSSION

In this section, NNMPC algorithm was implemented to control the temperature of MA removal reactor and the controller performance in set-point tracking and disturbance rejection was investigated compared with conventional PID controller.

Considering that no definite criteria provided in the choice of the prediction horizon for nonlinear system, closed loop simulations were carried out for step tracking with different prediction horizons in Fig.9, in order to select the appropriate value for the prediction horizon. Obviously, the prediction horizon of 27 provides most satisfactory control performance from Fig.9.

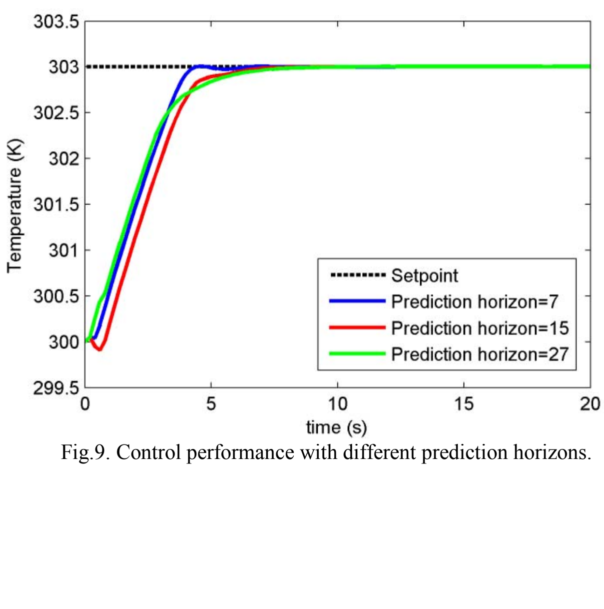

Fig.9. Control performance with different prediction horizons.

Similarly, the simulations to selecting the value control horizon were carried out. It was obviously observed that the control horizon value of 15 provides most satisfactory control performance from in Fig.10.

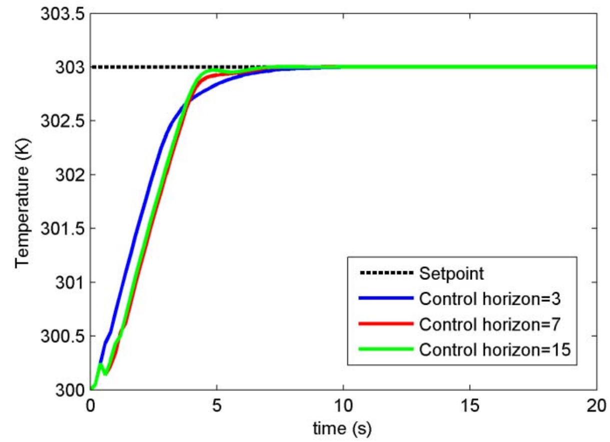

Fig.10. Control performance with different control horizons.

Fig.11 shows a comparison of the MA removal reactor temperature responses to a series of set-point changes due to the NNMPC and PID controllers. Initially, the coolant starts circulating at the rate 2L/min, at the same time, 100 L wastewater containing MA at the temperature of 310 K and the mixed bacteria strains were charge into the MA removal reactor and the initial temperature of the reactor was 300 K. The controlled temperature of the reactor was set 302 K at time100s, and 303.5 K at time 200 s. The control response obtained from Fig.11 shown that NNMPC was ideal with smaller overshoot and shorter settling times in comparison with the PID controller. In this work, the Cohen-Coon method was used for tuning the PID controller and the control setting for the PID controller was shown in TABLE IV. Besides, IAE (integrated absolute error) and ISE (integrated squared error) were employed to compare the performances of NNMPC and PID controllers quantitatively in TABLE V.

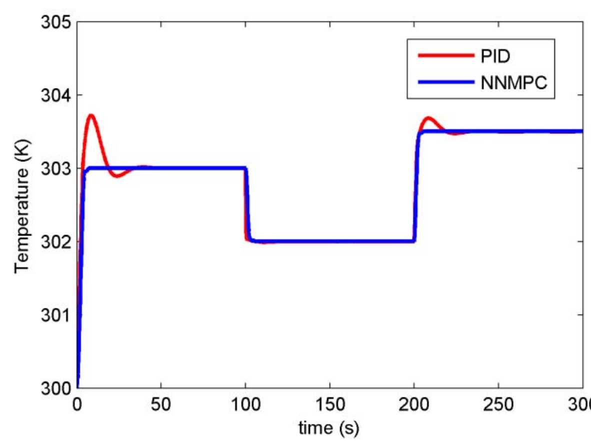

Fig.11. Control performance using NNMPC and PID controller.

TABLE IV
PARAMETERS FOR PID CONTROLLER

PID parameters	Value
Proportional constant	-15.12
Integral constant	0.44
Derivative constant	5.47

TABLE V
VALUE OF ISE AND IAE

Method	ISE	IAE
NNMPC	396.2648	707.3366
PID	521.9249	861.9722

Obviously, the error of NNMPC is smaller and the NNMPC provides more satisfactory control effect. In order to check the stability of NNMPC of MA removal reactor against process disturbances, another set of experiments were conducted. Fig.12 shown the control effect under the disturbance made by changing the temperature of wastewater containing MA from 310 K to 308 K at time 100 s. The simulation results shown in Fig.12 depicted that the controlled reactor temperature increased a little away from the set-point value then was driven back to track the set-point value faster in comparison with the PID controller.

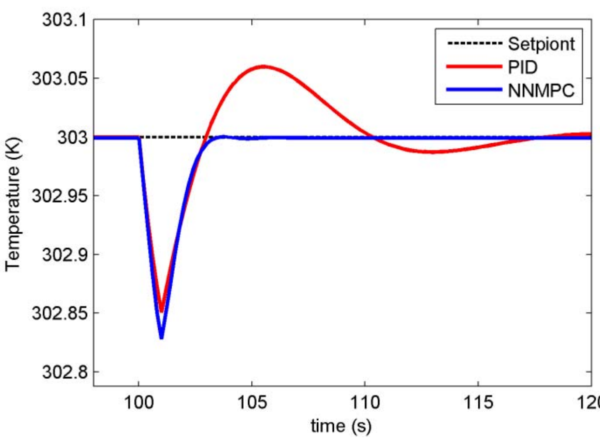

Fig.12. NNMPC and PID controller under disturbance made by changing the temperature of wastewater containing MA.

Similar procedure was performed under the disturbance made by changing the flow rate of wastewater containing MA from 1 L/min to 1.5L/min at time 100 s in Fig.13 and NNMPC provided stronger ability to reject disturbances in comparison with the PID controller.

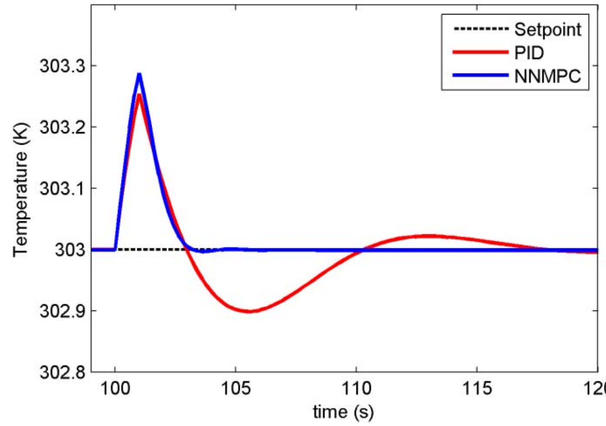

Fig.13. NNMPC and PID controller under disturbance made by changing the flow rate of wastewater containing MA.

VI. CONCLUSION

In this paper, the application of neural network based model predictive control strategy for controlling methylamine removal reactor is presented, which is to cover the gap between theoretical and practical control studies for the MA removal reactor. NNMPC shows better performance both in set-point tracking and disturbance rejection on the temperature control of MA removal reactor in comparison with the conventional PID controller. This study highlights the significance of using nonconventional system identification techniques and advanced control strategies for the control of complex MA removal reactor.

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