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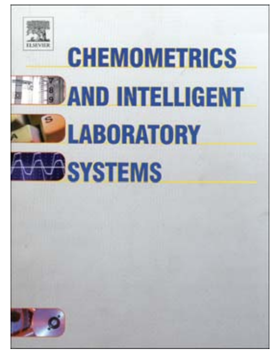

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Predictive control optimization based PID control for temperature in an industrial surfactant reactor

Ridong Zhang[a,b], Sheng Wu[a], Renquan Lu[a], Furong Gao[b*]

[a] *Information and Control Institute, Hangzhou Dianzi University, Hangzhou 310018,P R China*

[b] *Department of Chemical and Biomolecular Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong*

Abstract: Due to the character of nonlinearity, uncertainties, time delays and so on in the industrial reactors, the performance of proportional-integral-derivative (PID) control cannot always achieve the desired effect. Model predictive control (MPC) is a useful control strategy in the fact that the process models do not need to be accurately known. However, limited by the cost, hardware and so on, the application of MPC is less convenient than PID. In this paper, the temperature control in an industrial surfactant reactor is studied, where an improved PID controller optimized by extended non-minimal state space model predictive control (ENMSSMPC) framework is employed. The temperature in the surfactant reactor is first modeled as a typical step-response model and then a corresponding improved state space transformation with subsequent MPC design is done. The overall strategy combines the advantages of both PID's simple structure and MPC's good control performance. The proposed method is compared with traditional PID and MPC controllers and results show that it provides improved performance.

Keywords: Surfactant reactors, PID control, model predictive control, state space models, ensemble performance

Corresponding author: Tel: +852-2358-7139
E-mail address: kefgao@ust.hk

1. Introduction

Surfactant is necessary in our life, and its application can be found in most petro/chemical industries. It can be used for the production of dyestuffs, textiles, plastics and so on, besides, it also plays a significant role in the environmental protection, where it is transformed into the oil dispersants [1-2]. With the drastic development of economy, the use of surfactants also increases. In these surfactants, nonionic surfactants are the protagonist we will consider in this study, which have excellent cold water solubility and are effective over a large PH range. In order to satisfy the growing market need, the control performance associated with the productivity should be improved.

Industrial reaction processes are nonlinear with uncertainties and time delays, which make the control task difficult [3-4]. Even so, several researchers have attempted to propose effective methods to improve process operation. Muller, et al. [5] proposed an MPC algorithm for switched nonlinear systems under average dwell-time switching signals and applied it to a continuous stirred-tank reactor with two different modes of operation. Ho, et al. [6] proposed an adaptive predictive model-based control strategy for the control of production rate and temperature in a fluidized reactor. A decentralized versus centralized control strategy is put forward for the temperature regulation in an industrial chemical reactor by Petit and Del Vecchio [7]. Karer, et al. [8] proposed a self-adaptive predictive functional control for the temperature in an exothermic batch reactor. Aumi and Mhaskar [9] designed a computationally efficient nonlinear robust MPC for the control of a fed-batch reactor. Other researchers have also proposed effective control approaches for industrial reactors [10-19].

Many PID controllers based on nonlinear optimization are also proposed for diverse applications. Rani, et al. [20] proposed a modified genetic algorithm for the multi-objective optimization of PID controller parameters and tested it in a rotary inverted pendulum system. A robust self-learning proportional-integral-derivative (RSPID) control system design for nonlinear systems was proposed by Lin, et al. [21] and a particle swarm optimization (PSO) algorithm was also adopted to search the optimal learning-rates of PID adaptive gains, and finally a two-link manipulator and a chaotic system were examined to illustrate the effectiveness of the proposed control algorithm. A novel Artificial Intelligence (AI) technique known as Ant Colony Optimization (ACO) was used for optimal tuning of PID controller by Omar, et al. [22] and a reheat thermal system was tested for the effectiveness of the proposed technique. A fixed-order controller design method which only uses frequency responses was proposed by Doi, et al. [23], and the proposed method can derive a controller satisfying the control performance with non-linear optimization. Some fuzzy strategies based PID are also proposed [24-26].

The complex chemical reaction in the reactor is hard to predict, which reveals that the process model may be time-varying and requires a good robust controller against the model/plant mismatches. Disturbances caused by the temperature or pressure change taking place in the chemical reaction cannot be avoided neither. The production of surfactant needs an appropriate condition under which the reaction takes place. In order to improve the productivity and save energy, good performance for disturbance rejection is also needed for the control method.

Summarizing all the characteristics the controller should contain, a novel PID controller optimized by ENMSSMPC is proposed for the industrial surfactant reactor in this study. The new PID controller inherits the simple structure of conventional PID controller and the performance of ENMSSMPC and shows the following advantages:

Firstly, MPC is a useful algorithm in dealing with complicated processes, especially the processes with time delays and uncertainties [27-28]. The low requirement of accurate process models makes MPC effective in the industrial reaction processes. ENMSSMPC is a new MPC approach proposed by Zhang, et al. [29] where tracking and disturbance rejection performance can be improved. In terms of the difficulties mentioned above, ENMSSPC can handle them. Secondly, PID control is the most widely used control strategy in practice since MPC methods have more complicated structures and require higher costs [30-31]. The proposed PID controller optimized by ENMSSPC solves the problem and finds a compromise between them. In this study, the control law of PID controller is introduced to the framework of ENMSSMPC algorithm, and the parameters of PID control are obtained by optimizing the cost function of ENMSSMPC algorithm. The simple structure as traditional PID controller and good control performance as ENMSSPC in the new PID controller will be meaningful for practical reaction processes.

In order to verify the performance of the proposed PID controller, a surfactant reactor is considered as a case study and the PID controllers tuned by the typical Ziegler-Nichols (Z-N) method, Tyreus-Luyben (T-L) method, inner model control (IMC) method [32-34] and standard MPC are adopted for comparisons.

2. The Process Description

The sketch of the surfactant reactor is given in Fig. 1. Firstly, the nonylphenol and hydroxide (catalyst) are fed into the reactor and heated to the reaction temperature, then ethylene oxide (EO) is added slowly to react with the nonylphenol under the liquid phase. Higher temperature and partial pressure of EO will increase the reaction rate, however, it is not the case that the higher the better. When the upper temperature or pressure is exceeded, there will be an adverse effect on the product. If there is insufficient removal of heat generated from the reactions, a high concentration of EO in the reactor may lead to a run-away reaction. Besides, security should be taken into account. To maintain the process operation at its optimum conditions, the temperature and pressure must be controlled. Here the pressure can be an indirect measurement of concentration in reactor as it is a function of concentration and temperature. A sharp rise in the pressure occurs if there is excessive heat generation or a high concentration in the reactor. The reactor temperature is controlled by regulating the bypass valve of the recirculation fluid and the heat is removed from the process through a shell and tube heat exchanger. On the other side, the pressure of the reactor is affected directly by the density of the EO and the reactor temperature. The more EO is fed into the reactor, the higher temperature and pressure will be. Thus temperature is required to be controlled accurately and efficiently; here the EO feed is the manipulated variable.

3. The Process Model

In practice, a simple model is convenient for the controller design. First order plus dead time (FOPDT) model is the common form of process models, with which the design and computation of the controller will be simplified. The FOPDT model is shown as follows.

$$G(s)=\frac{Ke^{-\tau s}}{Ts+1} \tag{1}$$

where it has three parameters: K is the steady process gain, T is the time constant of the process and τ is the time delay.

The temperature control in the nonionic surfactant reactor is chosen as the control target. The temperature control system in the surfactant reactor is decomposed into two linear operating regimes because the changes in reaction kinetics and reactor volumes have strong effects on the process gain and time delay.

4. The New PID Controller

4.1 State space process model

After we obtain the FOPDT model of the temperature control system, it can be transformed into the difference equation model through sampling time T_s as follows.

$$y(k+1)+L_1 y(k)=S_{d+1}u(k-d) \tag{2}$$

where $y(k)$, $u(k)$ are the output and input of the controlled system at time instant k, respectively, $L_1=-e^{-T_s/T}$, $S_{d+1}=K(1+L_1)$ and $d=\tau/T_s$.

Add the back shift operator Δ to Eq. (2), it can be expressed as:

$$\Delta y(k+1)+L_1\Delta y(k)=S_{d+1}\Delta u(k-d) \tag{3}$$

The new state space vector $\Delta x_m(k)^{\mathrm{T}}$ is chosen as:

$$\Delta x_m(k)^{\mathrm{T}}=[\Delta y(k),\Delta u(k-1),\Delta u(k-2),\cdots,\Delta u(k-d)] \tag{4}$$

Then the corresponding state space model is derived as follows.

$$\begin{aligned} \Delta x_m(k+1) &= A_m \Delta x_m(k) + B_m \Delta u(k) \\ \Delta y(k+1) &= C_m \Delta x_m(k+1) \end{aligned} \tag{5}$$

where

$$A_m = \begin{bmatrix} -L_1 & 0 & \cdots & 0 & S_{d+1} \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

$$B_m = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^{\mathrm{T}}$$

$$C_m = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}$$

Define the expected output as $r(k)$, then the output tracking error is

$$e(k) = y(k) - r(k) \tag{6}$$

Combine Eq. (5) and Eq. (6), the formulation of $e(k+1)$ is as follows.

$$e(k+1) = e(k) + C_m A_m \Delta x_m(k) + C_m B_m \Delta u(k) - \Delta r(k+1) \tag{7}$$

Further formulate a new state variable $z(k)$:

$$z(k) = \begin{bmatrix} \Delta x_m(k) \\ e(k) \end{bmatrix} \tag{8}$$

Thus, the extended non-minimal state space model is as follows.

$$z(k+1) = Az(k) + B\Delta u(k) + C\Delta r(k+1) \tag{9}$$

where

$$A = \begin{bmatrix} A_m & 0 \\ C_m A_m & 1 \end{bmatrix}; B = \begin{bmatrix} B_m \\ C_m B_m \end{bmatrix}; C = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{10}$$

The 0 in Eq. (10) is a zero matrix with appropriate dimension.

4.2 Controller design

In this study, the control algorithm we choose to optimize the PID controller is MPC. In order to simplify the computation process, the control horizon M is chosen to be 1, then the future state variable based on Eq. (9) from sampling instant k is

$$Z = \varphi z(k) + \psi \Delta u(k) + \theta \Delta R \tag{11}$$

where

$$Z = \begin{bmatrix} z(k+1) \\ z(k+2) \\ \vdots \\ z(k+P) \end{bmatrix}; \varphi = \begin{bmatrix} A \\ A^2 \\ \vdots \\ A^P \end{bmatrix}; \theta = \begin{bmatrix} C & 0 & 0 & 0 & 0 \\ AC & C & 0 & 0 & 0 \\ A^2C & AC & C & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A^{P-1}C & A^{P-2}C & A^{P-3}C & \cdots & C \end{bmatrix}; \psi = \begin{bmatrix} B \\ AB \\ \vdots \\ A^{P-1}B \end{bmatrix}; \Delta R = \begin{bmatrix} \Delta r(k+1) \\ \Delta r(k+2) \\ \vdots \\ \Delta r(k+P) \end{bmatrix}$$

$$r(k+i) = \alpha^i y(k) + (1-\alpha^i)c(k)$$

Here P is the prediction horizon, α is the smoothing factor, and $c(k)$ is the set-point at time instant k .

The cost function $J(k)$ in this study is

$$\min J(k) = Z^{\mathrm{T}} Q Z + \Delta u(k)^{\mathrm{T}} \omega \Delta u(k) \tag{12}$$

where $Q = block\ diag\{Q_1, Q_2, \cdots, Q_P\}$, ω is the control weighting coefficient.

Remark 1. From $Q_i\ (i = 1, 2, \cdots, P)$ in Q , Eq.(4) and Eq.(8), it is seen that Q_i has its elements as $Q_i = diag\{q_{i\,y1}, q_{i\,u1}, \cdots, q_{i\,ud}, q_{i\,e}\}$, where $q_{i\,y1}$, $q_{i\,u1}, \cdots, q_{i\,ud}$ and $q_{i\,e}$ are the weights on the process output changes, input changes and the output tracking error.

Remark 2. The larger $q_{i\,y1}$ is, the more smooth response of the process will be. However, the response will also be slower. For $q_{i\,u1}, \cdots, q_{i\,ud}$,we can ignore them (i.e., let them be zeros) because the cost function Eq.(12) has already considered placing weights on the input changes; $q_{i\,e}$ is generally set to be 1 because the output tracking error must be considered. This reveals that we should find a compromise between $q_{i\,y1}$ and $q_{i\,e}$ for acceptable closed-loop responses. And since $q_{i\,e}$ is fixed to be 1, the rest work is to tune $q_{i\,y1}$ for improved control performance.

The PID controller used in the proposed method is of an incremental form, whose formula can be presented as follows.

$$\begin{aligned} u(k) = u(k-1) + K_p(k)(e_1(k) - e_1(k-1)) + K_i(k)e_1(k) \\ + K_d(k)(e_1(k) - 2e_1(k-1) + e_1(k-2)) \end{aligned}$$

$$e_1(k) = c(k) - y(k) \tag{13}$$

where $K_p(k), K_i(k), K_d(k)$ are the proportional coefficient, the integral coefficient and differential coefficient at time instant k respectively, $e_1(k)$ is the error between the set-point and actual output value at time instant k.

Eq. (13) can be converted into the following form in order to simplify the computation process.

$$\begin{aligned}
&u(k) = u(k-1) + w(k)^{\mathrm{T}} E(k) \\
&w(k) = \left[w_1(k), w_2(k), w_3(k)\right]^{\mathrm{T}} \\
&w_1(k) = K_p(k) + K_i(k) + K_d(k) \\
&w_2(k) = -K_p(k) - 2K_d(k) \\
&w_3(k) = K_d(k) \\
&E(k) = \left[e_1(k), e_1(k-1), e_1(k-2)\right]^{\mathrm{T}}
\end{aligned} \tag{14}$$

From Eqs. (5)~(14) and take a derivative of the cost function $J(k)$, we can obtain the optimal control law

$$w(k) = -\frac{\psi^{\mathrm{T}} Q(\varphi z(k) + \theta \Delta R) E(k)}{(\psi^{\mathrm{T}} Q \psi + \omega) E(k)^{\mathrm{T}} E(k)} \tag{15}$$

Then $K_p(k), K_i(k), K_d(k)$ are calculated as follows

$$\begin{aligned}
&K_p(k) = -w_2(k) - 2K_d(k) \\
&K_i(k) = w_1(k) - K_P(k) - K_d(k) \\
&K_d(k) = w_3(k)
\end{aligned} \tag{16a}$$

It can be easily found from Eq. (15) that $w(k)$ will be infinite if $E(k)^{\mathrm{T}} E(k)$ is approximating zero, i.e., $K_p(k), K_i(k), K_d(k)$ will be infinite which is unrealistic when the control system has reached the steady state since $e_1(k)$ is close to zero. Thus, it is necessary to set a small permissible error limitation δ in which $K_p(k), K_i(k), K_d(k)$ are unchanged and remain as the same values as the previous sampling instant, and details are shown as follows.

$$\begin{aligned}
&\begin{cases} K_p(k) = K_p(k-1) \\ K_i(k) = K_i(k-1) \quad \cdots\cdots |e_1(k)| \le \delta \\ K_d(k) = K_d(k-1) \end{cases} \\
&\begin{cases} K_p(k) = -w_2(k) - 2K_d(k) \\ K_i(k) = w_1(k) - K_P(k) - K_d(k) \cdots\cdots |e_1(k)| > \delta \\ K_d(k) = w_3(k) \end{cases}
\end{aligned} \tag{16b}$$

The control input at sampling instant k is

$$u(k) = u(k-1) + K_p(k)(e_1(k) - e_1(k-1)) + K_i(k)e_1(k) + K_d(k)(e_1(k) - 2e_1(k-1) + e_1(k-2)) \tag{17}$$

Remark 3. Note that although the proposed design is a PID control strategy, its tuning differs from standard PID in the fact that the proposed PID adopts an MPC formulation procedure. By such MPC formulation, tuning of this PID controller is in fact transformed into finding suitable parameters for tuning the closed-loop performance of the MPC, which includes prediction optimization for improved control performance.

5. Case study: the temperature regulation in the industrial surfactant reactor

Here we mainly discuss one of the operating regimes and the temperature control system is modeled as

$$G(s) = \frac{2.8e^{-28s}}{1310s+1} \tag{18}$$

The model in Eq. (18) is obtained through frequency domain closed-loop identification method by identifying the relationship between the temperature and bypass valve signal.

5.1 Comparison between typical PID controllers

5.1.1 Model/plant match case

Firstly, the control performance of theses PID controllers is evaluated under the model/plant match cases. The set-point of the reactor temperature is changed from 0 to 1 at time instant $k=0$ for all the methods, besides, output disturbance with amplitude of -0.05 and input disturbance with amplitude of -5 are added to the process respectively. Here the permissible error limitation δ is set as 10^{-5}, which means that the parameters of proposed PID controller will be unchanged and remain as the same values as the previous time instant when the error between the given reactor temperature and actual temperature is less than 10^{-5}. The parameters of ENMSSMPC algorithm used to optimize PID controller and those of the PID controllers tuned by Z-N method, T-L method and IMC method are listed in Table 1.

Fig. 2 shows the responses under case 1. It can be easily found that the ensemble performance of the proposed PID controller is the best although all these methods deal with the set-point tracking and disturbance rejection well. Compared with the proposed method, Z-N method shows an unacceptable overshoot, and the recovery ability of T-L method and IMC-PID method under input disturbance and output disturbance are not acceptable, especially this is worse for the IMC-PID method. The responses of the proposed PID controller are smoother than the other three methods and show no overshoot and oscillation. On the other hand, the recovery time of the proposed method under disturbances is also the best, which, for T-L method, is too long.

5.1.2 Model/plant mismatched case

Uncertainties exist in practice inevitably, which cause model/plant mismatches. The test of control performance under model/plant mismatched cases will be more meaningful, here the parameters of the actual process are obtained through Monte Carlo simulation and are supposed that a maximum of 20% uncertainty from the nominal process model is resulted, whose parameters can be seen in Eq. (18) as $K = 2.8, T = 1310, \tau = 28$. At the same time, the three parameters are mismatched simultaneously to test the control performance of these PID controllers. The three cases of parameters uncertainty are generated as follows.

Case 2: the mismatched process parameters are estimated as $K = 3.1, T = 1452, \tau = 30$.

Case 3: the mismatched process parameters are estimated as $K = 2.5, T = 1187, \tau = 26$.

Case 4: the mismatched process parameters are estimated as $K = 2.6, T = 1153, \tau = 30$.

For these model/plant mismatched cases, the control parameters remain the same as in case 1.

Fig. 3-5 show the responses of these methods. From an overall perspective, the ensemble performance of the proposed PID controller is better than the other three PID controllers although all these methods can adapt to mismatched situations. In Fig. 3, the recovery time of T-L method in set-point tracking is not ideal, and Z-N method shows a tremendous overshoot, which may be unacceptable in practice. IMC-PID method and T-L method show a small overshoot, but their performance still loses to the proposed method because overshoot exists. The responses of the proposed method are smoother than the other three methods, and note that the disturbance rejection ability of the proposed method is also outstanding. The situations in Figs. 4 and 5 are like those in Fig. 3, where the ensemble performance of the proposed methods is the best. Z-N method shows a big overshoot, and meanwhile, T-L method and IMC method show the poor recovery ability under both input and output disturbances. The recovery time of T-L method in set-point tracking is also the longest. The computation burden is listed in Table.3, it is seen that the computation time of the proposed and those of the PID controllers do not differ too much.

5.2 Comparison with Standard MPC

In order to further verify the control performance of proposed method, a comparison with standard MPC is made. The set-point of the reactor temperature is changed from 0 to 1 at time instant $k=0$ for the two methods, besides, output disturbance with amplitude of -0.05 and input disturbance with amplitude of -5 are added to the process respectively. Here the permissible error limitation δ is set as 10^{-5}. The parameters of these two algorithms are listed in Table 2. Fig.6 shows the model/plant match case and Figs. 7-9 show the responses under three model/plant mismatches cases that are listed in section 5.1.2.

From an overall perspective, the ensemble performance of proposed method is better than standard MPC. In Fig. 6, the proposed method shows faster response than standard MPC, and the recovery ability of the proposed method is also improved compared with standard MPC. In Fig. 7, the proposed method also shows improved set-point tracking ability and disturbance rejection than standard MPC. In Figs. 8-9, the results are the same as in Fig. 7. Overall, the ensemble performance of the process has been improved by the proposed method. The computation time listed in Table.3 shows that the computation loads of the two MPC controllers do not differ too much.

6. Conclusion

A novel PID controller optimized by ENMSSMPC is proposed for the temperature regulation in the industrial surfactant reactor. Using the new PID controller, good performance can be obtained for the production of nonionic surfactants in the reactor, which can be seen from simulations of the case study.

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Appendix

An extension to MIMO systems

Here we suppose that the controlled system has v inputs and b outputs. The discrete model of the process under sampling time T_s is:

$$y(k+1)+G_1 y(k)+G_2(k-1)+\cdots+G_n y(k-n+1)$$
$$=T_1 u(k)+T_2 u(k-1)+\cdots+T_n u(k-n+1) \quad \text{(A1)}$$

where $y(k)=\left[y_1(k), y_2(k),\cdots, y_b(k)\right]^{\mathrm{T}}, u(k)=\left[u_1(k), u_2(k),\cdots, u_v(k)\right]^{\mathrm{T}}$.

Then this model is transformed into the following formulation by adding the back shift operator Δ:

$$\Delta y(k+1)+G_1\Delta y(k)+G_2\Delta y(k-1)+\cdots+G_n\Delta y(k-n+1)$$
$$=T_1\Delta u(k)+T_2\Delta u(k-1)+\cdots+T_n\Delta u(k-n+1) \quad \text{(A2)}$$

The new state space vector $\Delta x_m(k)^{\mathrm{T}}$ is chosen as:

$$\Delta x_m(k)^{\mathrm{T}}=[\Delta y(k)^{\mathrm{T}},\Delta y(k-1)^{\mathrm{T}},\cdots,\Delta y(k-n+1)^{\mathrm{T}},\Delta u(k-1)^{\mathrm{T}},\Delta u(k-2)^{\mathrm{T}},\cdots,\Delta u(k-n+1)^{\mathrm{T}}]$$

where the dimension of $\Delta x_m(k)$ is $v\times(n-1)+b\times n$, then the corresponding state space model is:

$$\begin{aligned}\Delta x_m(k+1)&=A_m\Delta x_m(k)+B_m\Delta u(k)\\ \Delta y(k+1)&=C_m\Delta x_m(k+1)\end{aligned} \quad \text{(A3)}$$

where

$$A_m=\begin{bmatrix} -G_1 & -G_2 & \cdots & -G_{n-1} & -G_n & T_2 & \cdots & T_{n-1} & T_n \\ I_b & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & I_b & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & I_b & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & I_v & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & I_v & 0 \end{bmatrix}$$

$$B_m=[T_1^{\mathrm{T}} \quad 0 \quad 0 \quad \cdots \quad 0 \quad I_v \quad 0 \quad 0]$$

$$C_m=[I_b \quad 0 \quad 0 \quad \cdots \quad 0 \quad 0 \quad 0 \quad 0]$$

, I_v and I_b are the unit matrix with dimension v and b, and 0 is a zero matrix with appropriate dimension.

Define the expected output as $r(k)$, and the output tracking errors is:

$$e(k)=y(k)-r(k) \quad \text{(A4)}$$

We can obtain the following equation by combing Eq. (A3) and Eq. (A4).

$$e(k+1) = e(k) + C_m A_m \Delta x_m(k) + C_m B_m \Delta u(k) - \Delta r(k+1) \tag{A5}$$

where $r(k)$ and $e(k)$ are matrices with dimension $b \times 1$.

Further formulate a new state variable $z(k)$:

$$z(k) = \begin{bmatrix} \Delta x_m(k) \\ e(k) \end{bmatrix} \tag{A6}$$

Thus, the extended non-minimal state space model is derived as follows.

$$z(k+1) = Az(k) + B\Delta u(k) + C\Delta r(k+1) \tag{A7}$$

where

$$A = \begin{bmatrix} A_m & 0 \\ C_m A_m & I_b \end{bmatrix}; B = \begin{bmatrix} B_m \\ C_m B_m \end{bmatrix}; C = \begin{bmatrix} 0 \\ -I_b \end{bmatrix} \tag{A8}$$

The 0 in Eq. (A8) is a zero matrix with appropriate dimension.

In order to simplify the computation, the control horizon M is chosen to be 1, then the future state variable based on Eq. (A7) from sampling instant k is

$$Z = \varphi z(k) + \psi \Delta u(k) + \theta \Delta R \tag{A9}$$

where

$$Z = \begin{bmatrix} z(k+1) \\ z(k+2) \\ \vdots \\ z(k+P) \end{bmatrix}; \varphi = \begin{bmatrix} A \\ A^2 \\ \vdots \\ A^P \end{bmatrix}; \theta = \begin{bmatrix} C & 0 & 0 & 0 & 0 \\ AC & C & 0 & 0 & 0 \\ A^2C & AC & C & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A^{P-1}C & A^{P-2}C & A^{P-3}C & \cdots & C \end{bmatrix}; \psi = \begin{bmatrix} B \\ AB \\ \vdots \\ A^{P-1}B \end{bmatrix}; \Delta R = \begin{bmatrix} \Delta r(k+1) \\ \Delta r(k+2) \\ \vdots \\ \Delta r(k+P) \end{bmatrix}$$

$$r(k+i) = \alpha^i y(k) + (1-\alpha^i)c(k)$$

P is the prediction horizon, α is the smoothing factor, and $c(k)$ is the set-point at time instant k.

The cost function $J(k)$ and the formula of PID used to be optimized are

$$\min J(k) = Z^{\mathrm{T}} Q Z + \Delta u(k)^{\mathrm{T}} \omega \Delta u(k) \tag{A10}$$

$$u_j(k) = u_j(k-1) + K_{pj}(k)(ess_j(k) - ess_j(k-1)) + K_{ij}(k) ess_j(k)$$

$$+K_{dj}(k)(ess_j(k)-2ess_j(k-1)+ess_j(k-2)),\ j=1,2,\cdots,v$$

$$ess_j(k)=c_j(k)-y_j(k) \tag{A11a}$$

Here $Q=block\ diag\{Q_1,Q_2,\cdots,Q_P\}$, ω is the control weighting matrix, $u_j(k)$ is the j item of $u(k)$, $ess_j(k)$ is the error between the set-point and the actual output, $K_{pj}(k)$, $K_{ij}(k)$ and $K_{dj}(k)$ are the proportional coefficient, the integral coefficient and differential coefficient at time instant k, respectively.

Eq. (A11) can be converted into the following form:

$$\begin{aligned}
&u_j(k)=u_j(k-1)+w_j(k)^{\mathrm{T}}E_j(k)\\
&w_j(k)=\left[w_{j1}(k),w_{j2}(k),w_{j3}(k)\right]^{\mathrm{T}}\\
&w_{j1}(k)=K_{pj}(k)+K_{ij}(k)+K_{dj}(k)\\
&w_{j2}(k)=-K_{pj}(k)-2K_{dj}(k)\\
&w_{j3}(k)=K_{dj}(k)\\
&E_j(k)=\left[ess_j(k),ess_j(k-1),ess_j(k-2)\right]^{\mathrm{T}}
\end{aligned} \tag{A11b}$$

Then $u(k)$ can be presented as follows.

$$u(k)=u(k-1)+w(k)^{\mathrm{T}}E(k) \tag{A12}$$

where

$$w(k)=\begin{bmatrix} w_1(k) & 0 & 0 & \cdots & 0\\ 0 & w_2(k) & 0 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & \cdots & 0 & w_{v-1}(k) & 0\\ 0 & 0 & \cdots & 0 & w_v(k)\end{bmatrix};E(k)=\begin{bmatrix}E_1(k)\\E_2(k)\\ \vdots\\ E_v(k)\end{bmatrix}$$

From Eqs. (A3)~(A12) and take a derivative of the cost function $J(k)$, we can obtain the optimal control law:

$$w(k)=-E(k)(\varphi z(k)+\theta\Delta R)^{\mathrm{T}}Q\psi(\psi^{\mathrm{T}}Q\psi+\omega)^{-1}(E(k)^{\mathrm{T}}E(k))^{-1} \tag{A13}$$

Then $K_{pj}(k),K_{ij}(k),K_{dj}(k)$ are calculated as follows:

$$\begin{aligned}
&K_{pj}(k)=-w_{j2}(k)-2K_{dj}(k)\\
&K_{ij}(k)=w_{j1}(k)-K_{pj}(k)-K_{dj}(k)\\
&K_{dj}(k)=w_{j3}(k)
\end{aligned} \tag{A14}$$

In order to unfeasible computation, here we also need to set a permissible error limitation vector δ in which the parameters are unchanged and remain as the same values as the previous sampling instant, and details are as follows.

$$\begin{cases} K_{pj}(k) = K_{pj}(k-1) \\ K_{ij}(k) = K_{ij}(k-1) \quad \cdots\cdots \left| ess_j(k) \le \delta_j \right| \\ K_{dj}(k) = K_{dj}(k-1) \end{cases}$$

$$\begin{cases} K_{pj}(k) = -w_{j2}(k) - 2K_{dj}(k) \\ K_{ij}(k) = w_{j1}(k) - K_{pj}(k) - K_{dj}(k) \cdots\cdots \left| ess_j(k) > \delta_j \right| \\ K_{dj}(k) = w_{j3}(k) \end{cases} \tag{A15}$$

References

1. Khuu, S. M., Rodriguez, J. A., Romagnoli, J. A., Ngian, K. F. (2000). Optimisation and control of an industrial surfactant reactor. *Computers & Chemical Engineering*, 24, (2), 863-870.

2. Coello, M. D., Aragon, C. A., Rodriguez-Barroso, R., Quiroga J. M. (2009). Non-ionic surfactant biodegradation in lab-scale activated sludge. *Environmental Technology*, 30, (13), 1391-1396.

3. Zhang, R. D., Gao, F. R. (2013). Multivariable decoupling predictive functional control with non-zero-pole cancellation and state weighting: Application on chamber pressure in a coke furnace, *Chemical Engineering Science*, 94: 30-43.

4. Perez-Polo, M. F., Perez-Molina, M. (2012). Saddle-focus bifurcation and chaotic behavior of a continuous stirred tank reactor using PI control. *Chemical Engineering Science*, 74, 79-92.

5. Muller, M. A., Martius, P., Allgower, F. (2012). Model predictive control of switched nonlinear systems under average dwell-time. *Journal of Process Control*, 22, (9), 1702-1710.

6. Ho, Y. K., Shamiri, A., Mjalli, F. S., Hussain, M. A. (2012). Control of industrial gas phase propylene polymerization in fluidized bed reactors. *Journal of Process Control*, 22, (6), 947-958.

7. Del Vecchio, D., Petit, N. (2005). Boundary control for an industrial under-actuated tubular chemical reactor. *Journal of Process Control*, 15, (7), 771-784.

8. Karer, G., Skrjanc, I., Zupancic, B. (2008). Self-adaptive predictive functional control of the temperature in an

exothermic batch reactor. *Chemical Engineering and Processing: Process Intensification*, 47, (12), 2379-2385.

9. Aumi, S., Mhaskar, P. (2010). Robust model predictive control and fault handling of batch processes. *AICHE Journal*, 57, (7), 1796-1808.

10. Pérez-Polo, M. F., Pérez-Molina, M. (2013). Increasing the reactant conversion through induced oscillations in a continuous stirred tank reactor by using PI control. *Journal of Process Control*, 23, (5), 778-792.

11. Houska, B., Logist, F., Van Impe, J., Diehl, M. (2012). Robust optimization of nonlinear dynamic systems with application to a jacketed tubular reactor. *Journal of Process Control*, 22, (6), 1152-1160.

12. Diaz-Salgado, J., Alvarez, J., Schaum, A., Moreno, J. A. (2012). Feedforward output-feedback control for continuous exothermic reactors with isotonic kinetics. *Journal of Process Control*, 22, (1), 303-320.

13. Gharaghani, M., Abedini, H., Parvazinia, M. (2012). Dynamic simulation and control of auto-refrigerated CSTR and tubular reactor for bulk styrene polymerization. *Chemical Engineering Research & Design*, 90, (10), 1540-1552.

14. Flores-Tlacuahuac, A., Morales, P., Rivera-Toledo, M. (2012). Multiobjective nonlinear model predictive control of a class of chemical reactors. *Industrial & Engineering Chemistry Research*, 51, (17), 5891-5899.

15. Lucia, S., Finkler, T., Engell, S. (2013). Multi-stage nonlinear model predictive control applied to a semi-batch polymerization reactor under uncertainty. *Journal of Process Control*, 23, (9), 1306-1319.

16. Wali, W.A., Al-Shamma'a, A.I., Hassan, K. H., Cullen, J. D. (2012). Online genetic-ANFIS temperature control for advanced microwave biodiesel reactor. *Journal of Process Control*, 22, (7), 1256-1272.

17. Aksikas, I., Mohammadi, L., Forbes, J. F., Belhamadia, Y., Dubljevic, S. (2013). Optimal control of an advection-dominated catalytic fixed-bed reactor with catalyst deactivation. *Journal of Process Control*, 23, (10), 1508-1514.

18. Hoang, H., Couenne, F., Jallut, C., Gorrec, Y. L. (2012). Lyapunov-based control of non isothermal continuous

stirred tank reactors using irreversible thermodynamics.*Journal of Process Control*, 22, (2), 412-422.

19. Shenoy, A.V., Prakash, J., Prasad, V., Shah, S.L., McAuley, K.B. (2013). Practical issues in state estimation using particle filters: Case studies with polymer reactors.*Journal of Process Control*, 23, (2), 120-131.

20. Rani, M. R., Selamat, H., Zamzuri, H., Ibrahim, Z. (2012). Multi-objective optimization for PID controller tuning using the global ranking genetic algorithm. *International Journal of Innovative Computing, Information and Control*, 8, (1A), 269-284.

21. Lin, C. M., Li, M. C., Ting, A. B., Lin, M. H. (2011). A robust self-learning PID control system design for nonlinear systems using a particle swarm optimization algorithm. *International Journal of Machine Learning and Cybernetics*, 2, (4), 225-234.

22. Omar, M., Soliman, M., Abdel Ghany, A. M., Bendary, F. (2013). Ant colony optimization based PID for single area load frequency control. *2013 5th International Conference on Modeling, Identification and Control*, 119-123.

23. Doi, A., Yubai, K., Yashiro, D., Hirai, J. (2013). Design of a PID controller based on H infinity loop shaping method using frequency responses. *2013 13th International Conference on Control, Automation and Systems*, 966-969.

24. Savran, A. (2013). A multivariable predictive fuzzy PID control system. *Applied Soft Computing*, 13, (5), 2658-2667.

25. Sharma, R., Rana, K. P. S., Kumar, V. (2014). Performance analysis of fractional order fuzzy PID controllers applied to a robotic manipulator. *Expert Systems with Applications*, 41, (9), 4274-4289.

26. Dastranj, M. R., Moghaddas, M., Afghu, S. S., Rouhani, M. (2011). PID control of inverted pendulum using particle swarm optimization (PSO) algorithm. *2011 IEEE 3rd International Conference on Communication Software and Networks*, 575-578.

27. Zhang, R.D., Wang, S.Q. (2008). Support vector machine based predictive functional control design for output temperature of coking furnace. *Journal of Process Control*,18(5):439-448.

28. Qin, S. J., Badgwell, T. A. (2003). A survey of industrial model predictive control technology. *Control Engineering Practice*, 11, (7), 733-764.

29. Zhang, R. D., Xue, A. K., Wang, S. Q., Ren, Z. Y. (2011). An improved model predictive control approach based on extended non-minimal state space formulation. *Journal of Process Control*, 21, (8), 1183-1192.

30. Xu, M., Li, S. Y., Cai, W. J. (2005). Practical receding-horizon optimization control of the air handling unit in HVAC systems. *Industrial & Engineering Chemistry Research*, 44, (8), 2848-2855.

31. Zhang, R. D., Xue, A. K., Wang, S. Q. (2011). Modeling and nonlinear predictive functional control of liquid level in a coke fractionation tower, *Chemical Engineering Science*, 66(23)：6002-6013.

32. Ziegler, J. G., Nichols, N.B., Rochester, N. Y. (1942). Optimum settings for automatic controllers. *Transactions of American Society of Mechanical Engineers*, 759-768.

33. Luyben, W. L. (1996). Tunning proportional-integral-derivative controllers for integrator/dead time processes. *Industrial & Engineering Chemistry Research*, 35, (10), 3480-3483.

34. Bequette, B. W. (2003). Process Control: Modeling, Design and Simulation. Prentice Hall, Upper Saddle River, NJ.

Figure &Table Captions:

Fig.1. Schematic structure of the surfactant reactor.

Fig.2. Closed-loop servo response under case 1.

Fig.3. Closed-loop servo response under case 2.

Fig.4. Closed-loop servo response under case 3.

Fig.5. Closed-loop servo response under case 4.

Fig.6. Closed-loop servo response under case 1.

Fig.7. Closed-loop servo response under case 2.

Fig.8. Closed-loop servo response under case 3.

Fig.9. Closed-loop servo response under case 4.

Table 1a. Tuning Parameters for Traditional PID Controllers.

Table 1b. Tuning Parameters for the Proposed PID Controller.

Table 2. Tuning Parameters for Servo Problem.

Table 3. Computation Time under Case 1-4 (1000 steps)

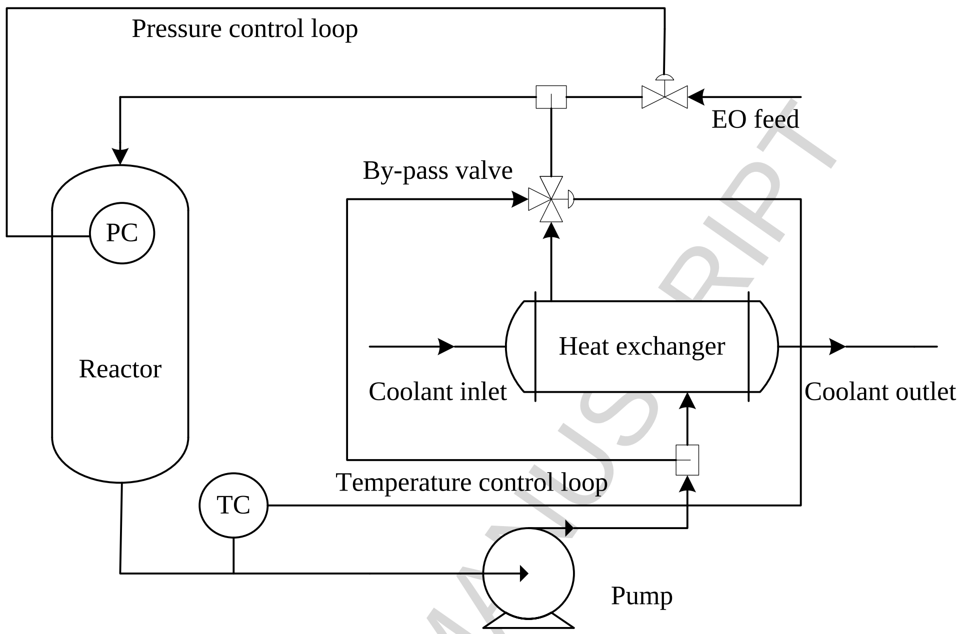

Fig. 1. Schematic structure of the surfactant reactor

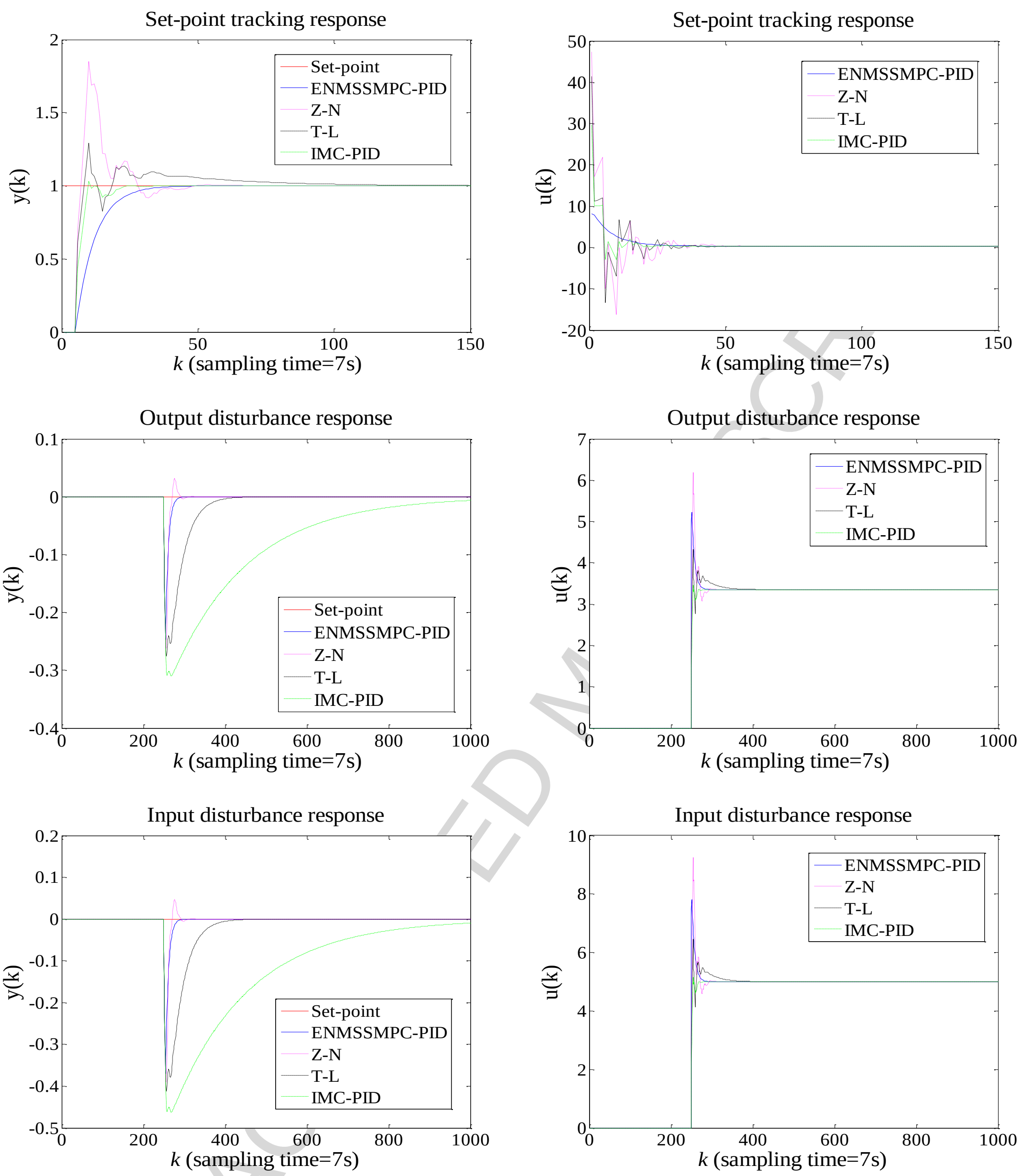

Fig. 2. Closed-loop servo response under case 1.

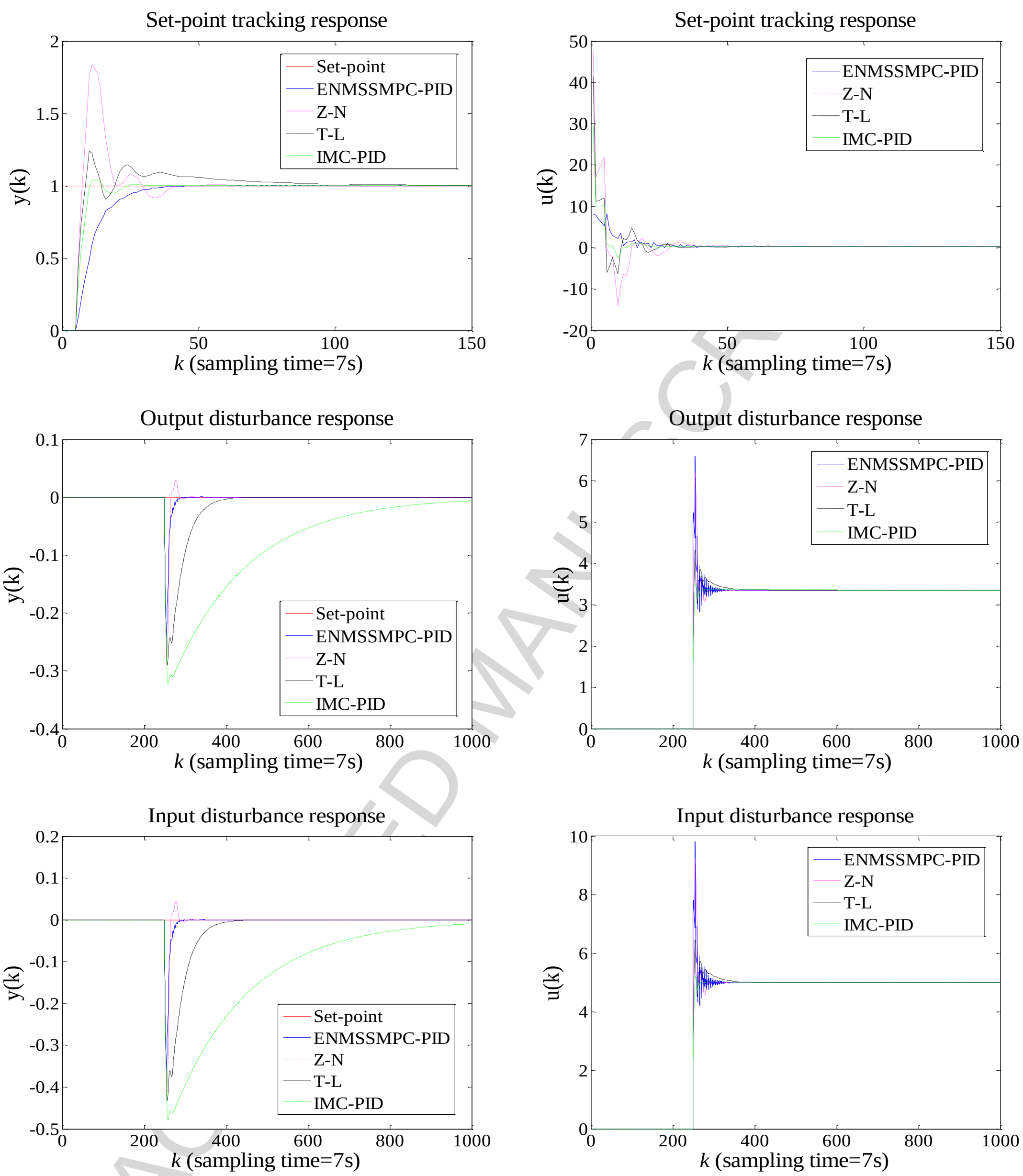

Fig. 3. Closed-loop servo response under case 2.

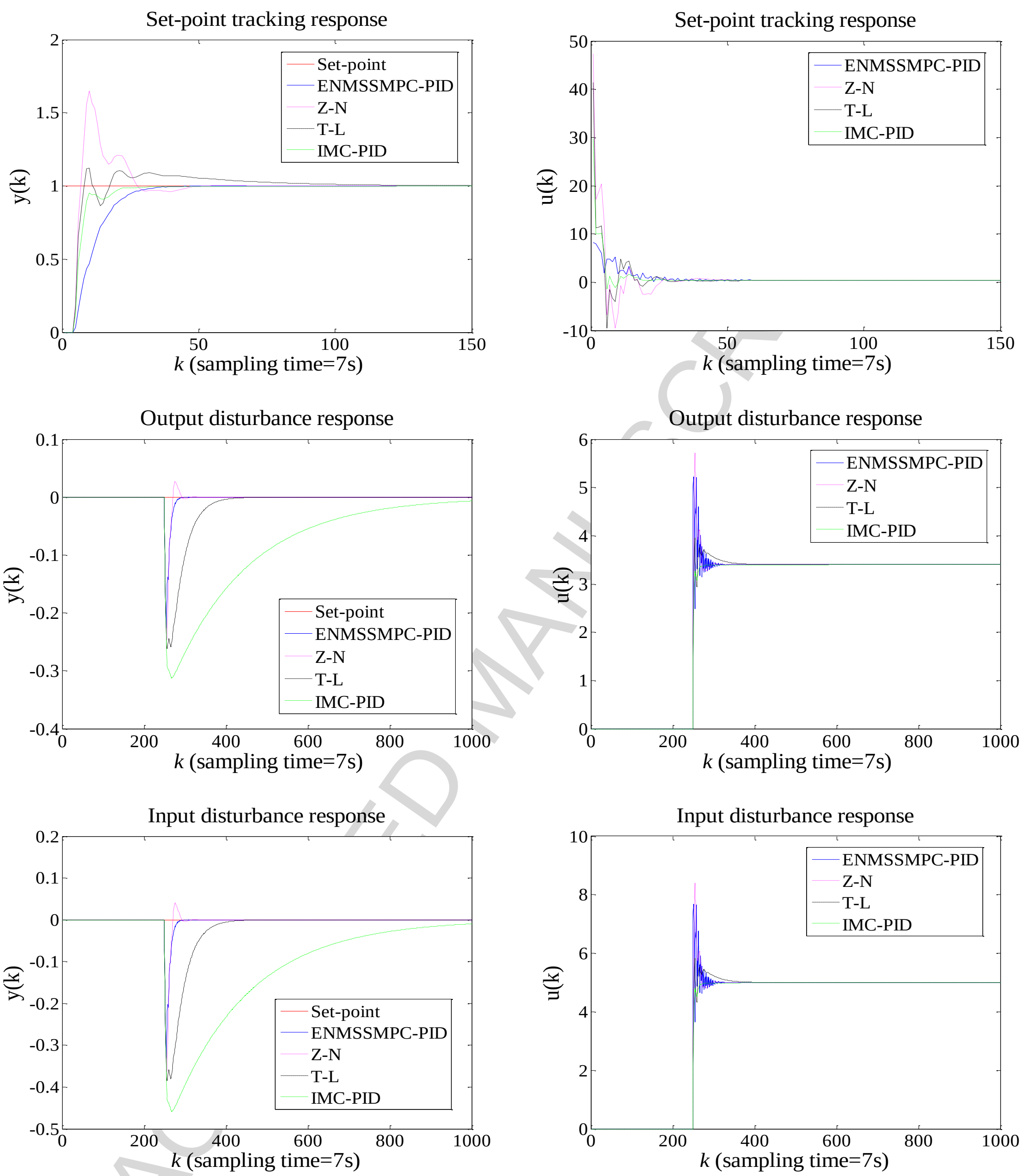

Fig. 4. Closed-loop servo response under case 3.

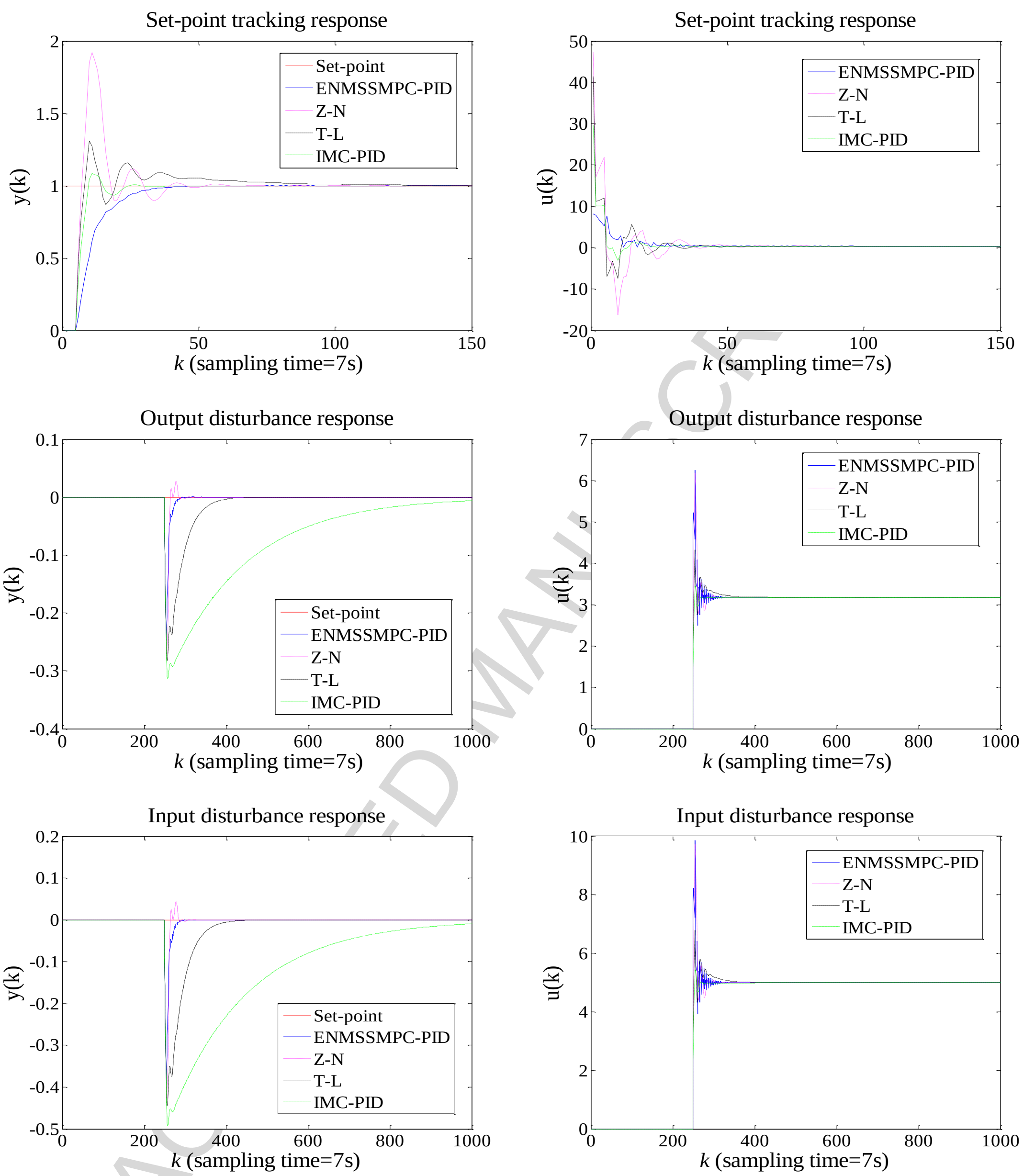

Fig. 5. Closed-loop servo response under case 4.

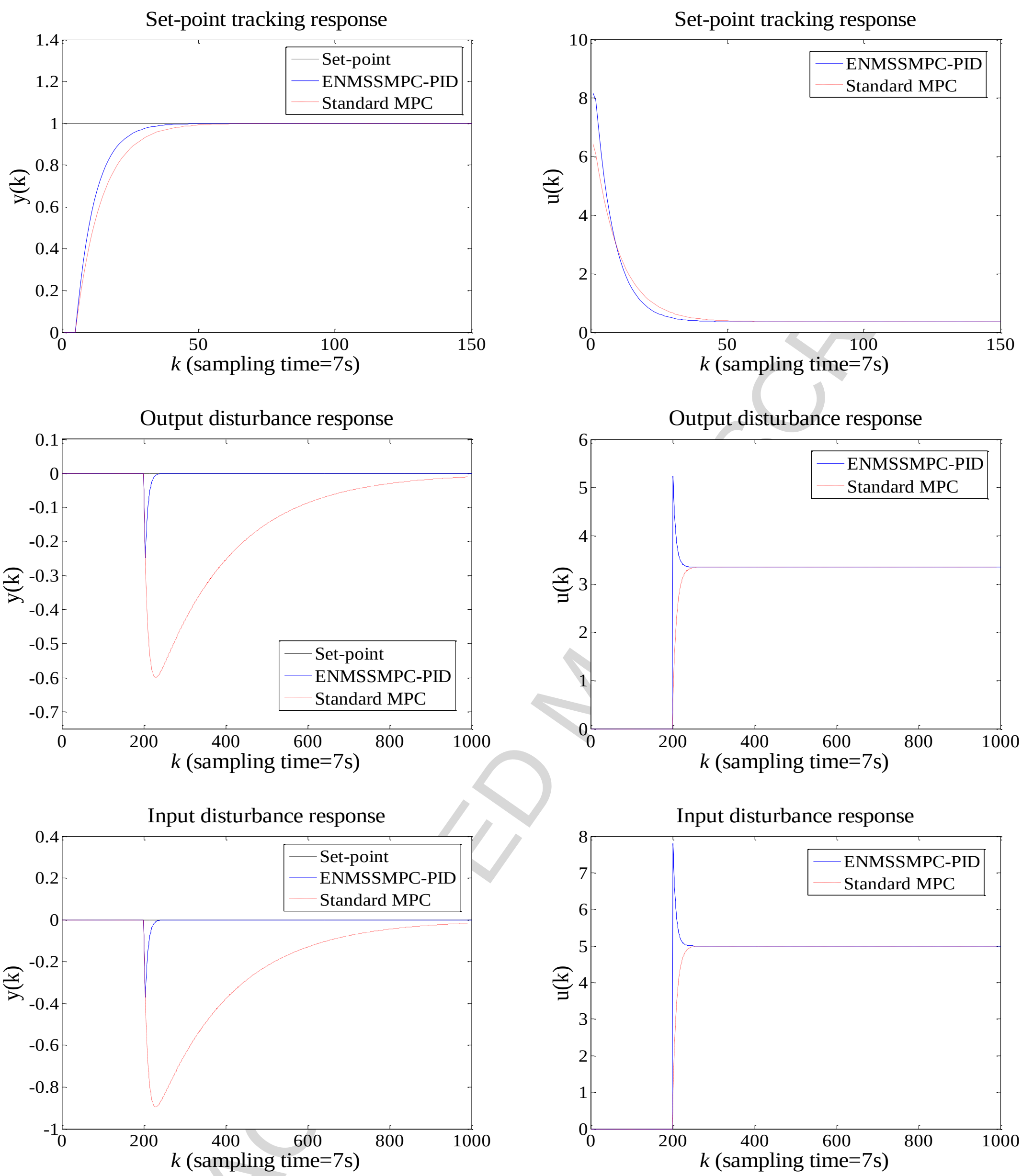

Fig. 6. Closed-loop servo response under case 1.

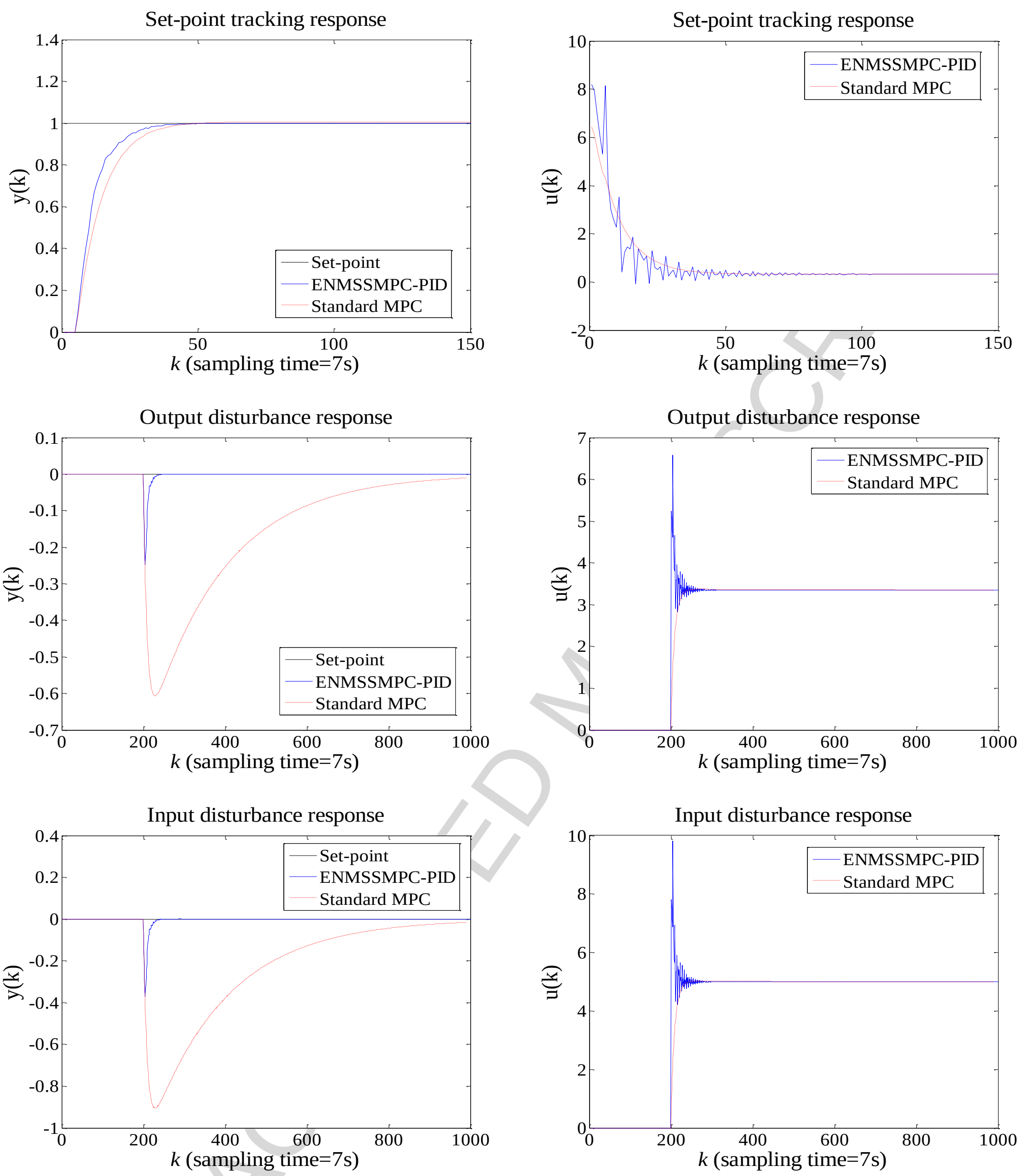

Fig. 7. Closed-loop servo response under case 2.

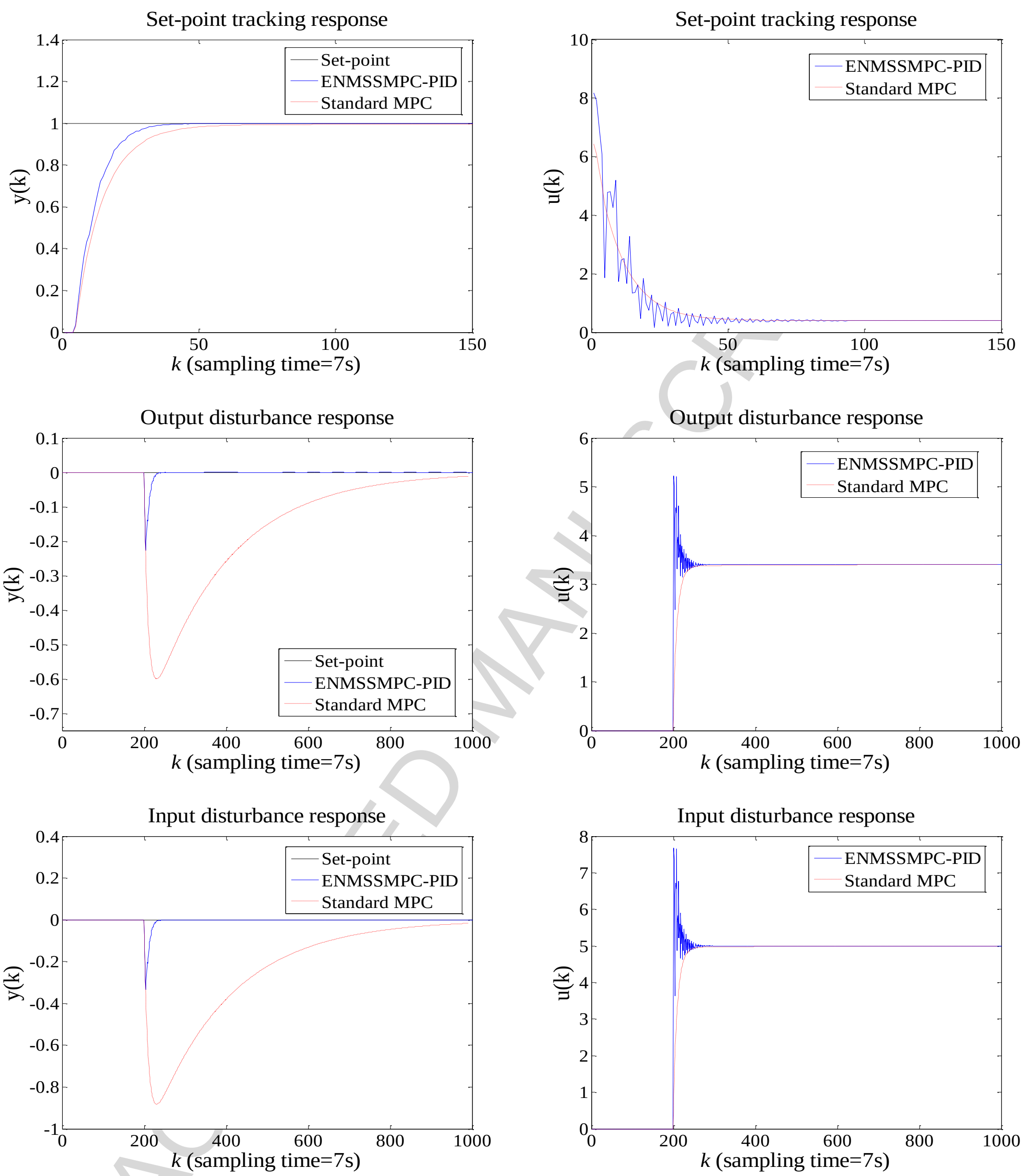

Fig. 8. Closed-loop servo response under case 3.

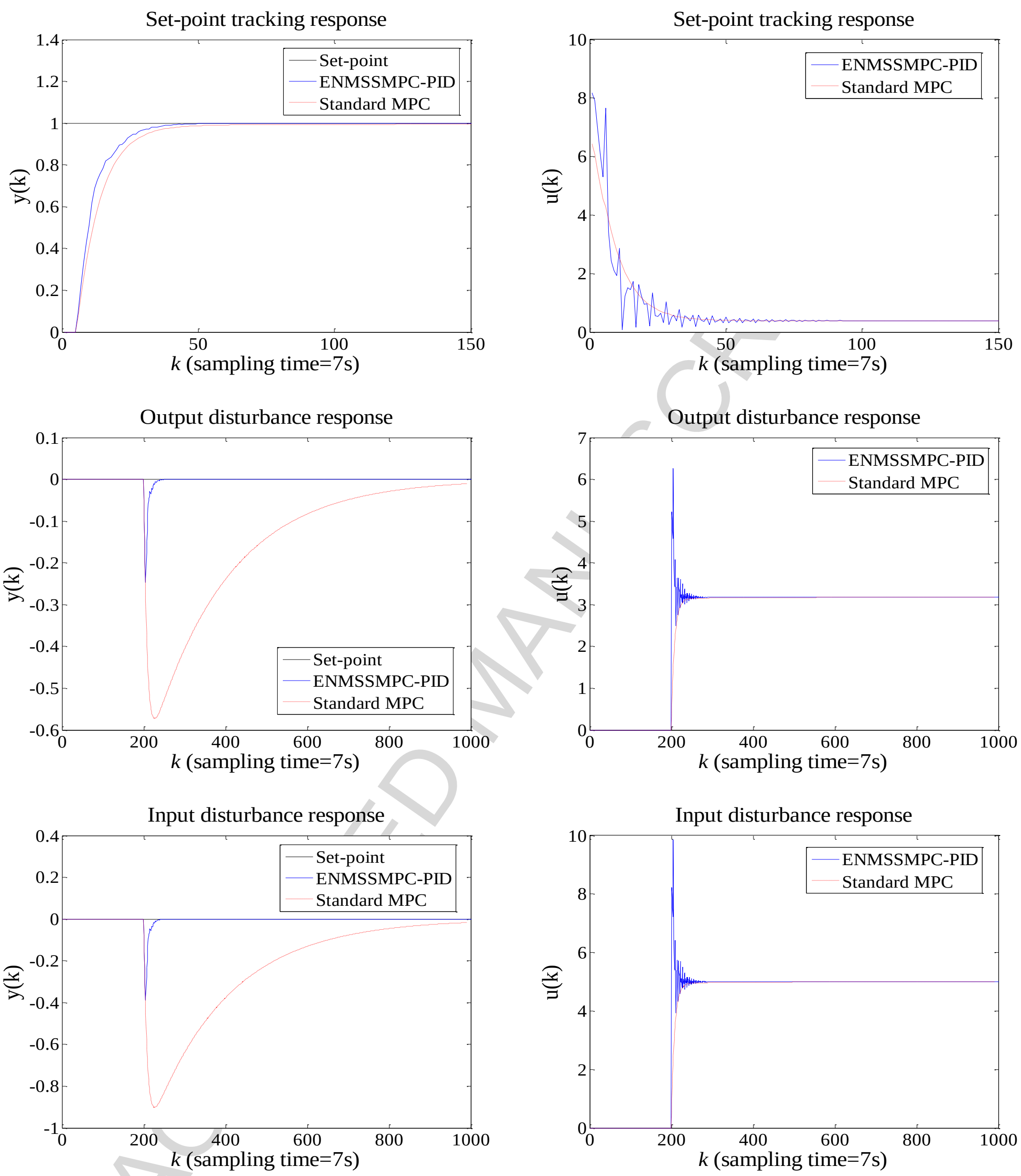

Fig. 9. Closed-loop servo response under case 4.

Table 1a. Tuning Parameters for Traditional PID Controllers

Parameters	Z-N	T-L	IMC-PID
K_p	14.07	10.66	9.93
T_i	63	277	1324
T_d	15.75	20	13.85

Table 1b. Tuning Parameters for the Proposed PID Controller

Parameters	Proposed
P	15
M	1
α	0
Q_i (i=1,2..., P)	diag(0,0,0,0,0,1)
ω	0.01

Table 2. Tuning Parameters for MPC

Parameters	ENMSSMPC-PID	Standard MPC
P	15	15
M	1	1
α	0	0
Q_i (i=1,2..., P)	diag(0,0,0,0,0,1)	1
ω	0.01	0.01

Table 3. Computation Time under Case 1-4 (1000 steps)

Case	Item	Set-point tracking	Output disturbance	Input disturbance
Case 1	ENMSSMPC-PID	1.152102s	1.213797s	1.211926s
	Standard MPC	0.983762s	0.988927s	0.986960s
	Z-N	0.968220s	0.977588s	0.981741s
	T-L	0.979323s	0.981165s	0.988695s
	IMC-PID	0.971062s	0.981615s	0.980970s
Case 2	ENMSSMPC-PID	1.260348s	1.356497s	1.357371s
	Standard MPC	1.110673s	1.117407s	1.118419s
	Z-N	1.096386s	1.103427s	1.108669s
	T-L	1.091941s	1.109593s	1.104503s
	IMC-PID	1.102228s	1.108527s	1.105564s
Case 3	ENMSSMPC-PID	1.292652s	1.334997s	1.354343s
	Standard MPC	1.122575s	1.119580s	1.120663s
	Z-N	1.093399s	1.117162s	1.114895s
	T-L	1.113066s	1.118202s	1.107869s
	IMC-PID	1.102661s	1.114815s	1.116070s
Case 4	ENMSSMPC-PID	1.286820s	1.341344s	1.360283s
	Standard MPC	1.110397s	1.117931s	1.121654s
	Z-N	1.095261s	1.108308s	1.108366s
	T-L	1.103622s	1.103084s	1.107906s
	IMC-PID	1.102840s	1.110547s	1.101578s

Highlights

► A novel PID controller optimized by model predictive control (MPC) is proposed.

► The design is applied to temperature in the industrial surfactant reactor.

► Improved closed-loop control performance is achieved in terms of set-point tracking and disturbance rejection.