Adaptive Nonlinear Constrained Predictive Control of pH Neutralization in Fed-batch Bio-reactor

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Abstract: In this paper, an Adaptive Nonlinear Constrained Model Predictive Control (ANCMPC) is presented for a pH control in a fed-batch bio-reactor. The pH model is represented with Hammerstein Model. The static nonlinear part of Hammerstein model is described with the static pH model, and the dynamic linear part of the Hammerstein model is described with the CARIMA model. The parameters of the CARIMA model is estimated on-line with the input and output measurements of the system using a recursive least squares type of identification algorithm. The effectiveness of the proposed controller is shown through simulations.

Keywords: adaptive, nonlinear, constraint, model predictive control, pH neutralization, bio-reactor,Control Autoregulative Integrated Moving Average (CARIMA) and Hammerstein model

Nomenclature

h :	Tank level
S :	The area of the bio-reactor
q_1 :	Acid flow-rate
q_2 :	Buffer flow-rate
q_3 :	Base flow-rate
W_{ai} :	Reaction invariant of a charge related quantity of stream (i=1,2,3,4)
W_{bi} :	Reaction invariant of a carbonate ion related quantity of stream (i=1,2,3,4)
pK_1 :	Equilibrium constant
pK_2 :	Equilibrium constant
pH :	pH value of the medium
$u(k)$:	System input value q_3
$v(k)$:	Intermediate value in Hammerstein model
NL :	Nonlinear part of Hammerstein model
DL :	Dynamic linear part of Hammertein model
dt :	Sampling time
p :	The predictive horizon value
m :	The control horizon value
d :	The delay time

1. INTRODUCTION

The pH value of the medium has considerable influence on the growth and the metabolic activity of the microorganisms and cells. Contrarily, the pH value is not only affected by growth and production of microorganisms or cells, but also affected by added substrates. Firstly, a fermentation or culture cycle is divided into two phases: growth phase and production phase, and they have different pH value in process. Secondly, in a fed batch process, the substrates added into the bio-reactor usually have the different pH value and affect the stability of the pH value in the bio-reactor.

For the sake of maintaining the optimal conditions of growth and production, the optimal pH value must be kept. However, it is difficult to control the pH value of the medium with adequate performance due to its nonlinearities of titration and ambient effects as above.

In order to enhance the control performance of pH, there are serval works on pH control in literatures. Raymond A. Wright proposed an on-line identification and nonlinear controller for pH process[5]. R. Babuska et al. proposed a fuzzy self-tuning PI control of pH in fermentation[3]. Zhang Zhi-huan proposed a predictive controller based on multiple model for a pH nonlinear process[2]. S. -S. Yoon et al. proposed an indirect adaptive nonlinear controller for a pH process[1]. However, these pH control techniques suffer from one or more of the following shortcomings: (i) a process model with linear dynamics is employed; (ii) process nonlinearities are incompletely compensated; (iii) constraints of the system are not considered.

In this paper, in order to solve these problems, an adaptive nonlinear constrained model predictive controller based on Hammerstein model is proposed. In accordance with the nonlinear process of fed-batch bio-reactor, the system model of pH neutralization process is representable with Hammerstein model ([6] and [11]). It includes static nonlinear part and dynamic linear part. The static nonlinear part is described with the static model of the nonlinear pH model. The dynamic linear part is represented by the CARIMA model. The parameters of the CARIMA model are identified by using Recursive Least Square (RLS) algorithm on line. The simulation results show that the proposed controller can satisfactorily track the plant output to the reference pH value. It shows that the proposed controller has good performance with respect to the varying substrate feeding disturbance.

2. pH MODEL

The pH neutralization model is based on results from Henson and Seborg ([7] and [10]). Fig. 1 depicts a simplified schematic diagram of the considered pH neutralization process. The process consists of an acid stream q_1, buffer stream q_2 and base stream q_3. All three streams are mixed in the bio-reactor. The pH value pH of the bio-reactor is controlled by manipulating the acid and base flow rate. The pH neutralization model is as follows:

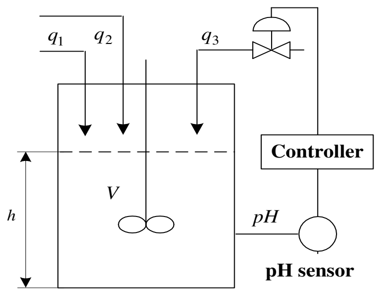

Fig. 1. The pH neutralization system

$$\dot{h} = \frac{1}{S}(q_1 + q_2 + q_3) \tag{1}$$

$$\dot{W}_{a_4} = \frac{1}{Sh}[(W_{a_1} - W_{a_4})q_1 + (W_{a_2} - W_{a_4})q_2 + (W_{a_3} - W_{a_4})q_3] \tag{2}$$

$$\dot{W}_{b_4} = \frac{1}{Sh}[(W_{b_1} - W_{b_4})q_1 + (W_{b_2} - W_{b_4})q_2 + (W_{b_3} - W_{b_4})q_3] \tag{3}$$

$$W_{b_4}\frac{1 + 2 \times 10^{pH_4 - pK_2}}{1 + 10^{pK1 - pH_4} + 10^{pH_4 - pK_2}} - 10^{-pH_4} + W_{a_4} + 10^{pH_4 - 14} = 0 \tag{4}$$

3. CONTROLLER DESIGN

In this section, the adaptive nonlinear constrained model predictive controller based on Hammerstein model is proposed. The block diagram of the ANCMPC system is shown in the Fig. 2. The thick line depicts the vector value, and the thin line depicts the scalar value.

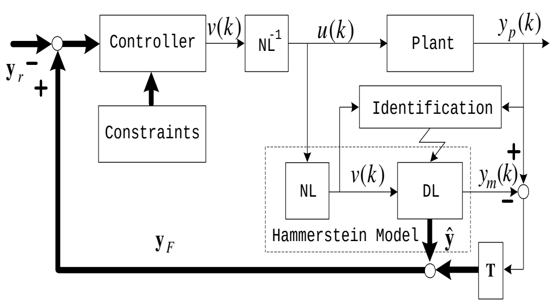

Fig. 2. The block diagram of the ANCMPC System

3.1. Hammerstein model

The plant is representable with the single input and single output (SISO) discrete-time Hammerstein model, which is consisted of two parts: a static nonlinear part NL and

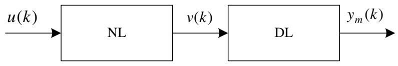

Fig. 3. The structure of the Hammerstein Model

a dynamic linear part DL (Fig. 3). The static nonlinear part NL is described with the static nonlinear pH model as follows[12]:

$$\frac{1}{Sh}[(W_{a_1} - W_{a_4})q_1 + (W_{a_2} - W_{a_4})q_2 + (W_{a_3} - W_{a_4})q_3] = 0 \tag{5}$$

$$\frac{1}{Sh}[(W_{b_1} - W_{b_4})q_1 + (W_{b_2} - W_{b_4})q_2 + (W_{b_3} - W_{b_4})q_3] = 0 \tag{6}$$

$$W_{b_4}\frac{1 + 2 \times 10^{pH_4 - pK_2}}{1 + 10^{pK1 - pH_4} + 10^{pH_4 - pK_2}} - 10^{-pH_4} + W_{a_4} + 10^{pH_4 - 14} = 0 \tag{7}$$

From equation ($5 \sim 7$), the static pH value pH_4 can be calculated and regarded as intermediate value $v(k)$ of Hammerstein model. Fig. 4 shows the static nonlinear characteristic of pH_4 to the input q_3 from equation ($5 \sim 7$). The

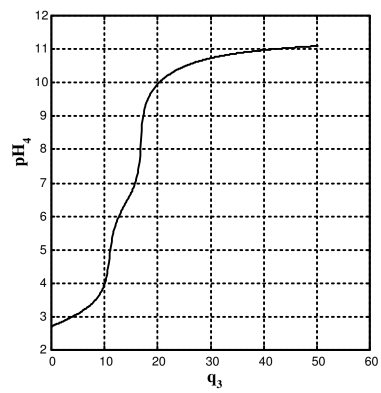

Fig. 4. The pH process static characteristic.

dynamic linear part of Hammerstein model is represented by a linear discrete-time model as follows:

$$A(z^{-1})y_m(k) = B(z^{-1})v(k-1) + \xi(k)/\Delta \tag{8}$$

where,

$$A(z^{-1}) = 1 + a_1 z^{-1} + \cdots + a_{n_a} z^{-n_a} \tag{9}$$

$$B(z^{-1}) = b_0 + b_1 z^{-1} + \cdots + b_{n_b} z^{-n_b} \tag{10}$$

$$\Delta = 1 - z^{-1} \tag{11}$$

and,

$y_m(k)$: The model output variable pH.
z^{-1} : The backward shift operator.
n_a : The power of $A(z^{-1})$.
n_b : The power of $B(z^{-1})$.
a_i : coefficients of $A(z^{-1})$.
b_i : coefficients of $B(z^{-1})$.
Δ : The unit difference operator.
$\xi(k)$: an uncorrelated random sequence.

3.2. Identification of the CARIMA model

The parameters of the linear part of Hammerstein model (CARIMA model) are identified by using Recursive Least Square (RLS) algorithm. Equation (8) is rewritten as following difference equation[9]:

$$\begin{aligned} y_p(k) &= -a_1 y_p(k-1) - a_2 y_p(k-2) - \cdots - a_{a_n} y_p(k - \\ &\quad n_a) + b_0 v(k-1) + \cdots + b_{n_b} v(k-1-n_b) + \xi(k) \\ &= \boldsymbol{\phi}^T(k)\boldsymbol{\theta} + \xi(k) \end{aligned} \quad (12)$$

where,

$$\begin{aligned} \boldsymbol{\phi}^T(k) &= [-y_p(k-1), \cdots, -y_p(k-n_a), v(k-1), \\ &\quad v(k-2), \cdots, v(k-n_b-1)], \\ \boldsymbol{\theta} &= [a_1, b_2, \cdots, b_0, \cdots, b_{n_b}]^T \end{aligned}$$

and,

$y_p(k)$ The plant output variable pH

$\boldsymbol{\phi}(k)$: Input output observational vector.

$\boldsymbol{\theta}$: The unknown vector.

Based on the n times observational values $\{y_p(i), n(i), i = 1, \cdots, N, N \leq n_a + n_b + 1\}$, the error $\epsilon(k)$ between the real value $y_p(k)$ and identified value $\hat{y}_E = \boldsymbol{\phi}^T(k)\hat{\boldsymbol{\theta}}$ at k time is as follows:

$$\epsilon(k) = y_p(k) - \boldsymbol{\phi}^T(k)\hat{\boldsymbol{\theta}} \quad = \boldsymbol{\phi}^T(k)(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + \xi(k) \quad (13)$$

and then, the parameters of the model are identified by using recursive least square method as follows:

$$\begin{aligned} \hat{\theta}(N) &= \hat{\theta}(N-1) + K(N)[y_p(N) \\ &\quad -\phi^T(N)\hat{\theta}(N-1)] \quad (14) \\ K(N) &= \frac{P(N-1)\phi(N)}{\rho + \phi^T(N)P(N-1)\phi(N)} \\ P(N) &= \frac{1}{\rho}[I - K(N)\phi^T(N)P(N-1)] \end{aligned}$$

where,

$\hat{\theta}$: The estimation value of θ.

ρ : The forgetting operator, $0.95 \leq \rho \leq 0.99$.

3.3. Optimal p^{th} step prediction

Based on predictive control theory, calculate the following Diophantine function[8],

$$E_j(z^{-1})A(z^{-1})\Delta + z^{-j}F_j(z^{-1}) = 1 \quad (15)$$

$$B(z^{-1})E_j(z^{-1} = G_j(z^{-j}) + z^{-1}H_j(z^{-1}) \quad (16)$$

where,

$j = 1, \cdots, p.$

The p^{th} step optimal predictive value is as follows:

$$\hat{\boldsymbol{y}} = \boldsymbol{G}\Delta\boldsymbol{v} + \boldsymbol{F}\boldsymbol{y}_m + \boldsymbol{H}\Delta v(k-1) \quad (17)$$

where,

$$\hat{\boldsymbol{y}} = [\hat{y}(k+1), \cdots, \hat{y}(k+p)]^T \quad (18)$$

$$\boldsymbol{y}_m = [y_m(k), \cdots, y_m(k-m+1)]^T \quad (19)$$

$$\Delta\boldsymbol{v} = [\Delta v(k), \Delta v(k+1), \cdots, \Delta u(k+m-1)]^T \quad (20)$$

$$\boldsymbol{F}^T = [F_1, \cdots, F_p] \quad (21)$$

$$\boldsymbol{H}^T = [H_1, \cdots, H_p] \quad (22)$$

$$\boldsymbol{G} = \begin{bmatrix} g_0 & 0 & 0 & 0 \\ g_1 & g_0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ g_{m-1} & g_{m-2} & \cdots & g_0 \\ \vdots & \vdots & \vdots & \vdots \\ g_{p-1} & g_{p-2} & \cdots & g_{p-m} \end{bmatrix} \quad (23)$$

The feedback value $\boldsymbol{y}_F$ is as follows:

$$\boldsymbol{y}_F = \hat{\boldsymbol{y}} + \boldsymbol{T}(y_p(k) - y_m(k)) \quad (24)$$

where,

$\boldsymbol{T}$: Transformation operator.

3.4. Optimal control input

The control law is derived based on the minimization of the cost function as follows:

$$J = E\{(\boldsymbol{y}_F - \boldsymbol{y}_r)^T(\boldsymbol{y}_F - \boldsymbol{y}_r) + \lambda\Delta\boldsymbol{v}^T\Delta\boldsymbol{v}\} \quad (25)$$

where,

$$\boldsymbol{y}_r = [y_r(k+1), \cdots, y_r(k+p)]^T$$

and,

$E\{\cdot\}$: Expectation.

λ : Scalar cost on the control increments.

Minimizing this cost equation, the optimal minimized input $v(k)$ without constraints can be calculated as follows:

$$\begin{aligned} \Delta\boldsymbol{v}(k) &= (\boldsymbol{G}^T\boldsymbol{G} + \lambda\boldsymbol{I})^{-1}\boldsymbol{G}^T(\boldsymbol{y}_r - \boldsymbol{F}\boldsymbol{y}_m \\ &\quad -\boldsymbol{H}\Delta v(k-1) - \boldsymbol{T}(y_p(k) - y_m(k))) \end{aligned} \quad (26)$$

The k^{th} step intermediate input $v(k)$ can be calculated as follows:

$$v(k) = v(k-1) + \Delta\boldsymbol{v}(1) \quad (27)$$

Using the inverse equation of the static nonlinear part of Hammerstein model (equation (5)∼ equation(7)), then, the optimal input $u(k)$ can be calculated without constraints as shown in Fig.3.

3.5. Constraints condition

Having stated the predictive control law, now consider the constraints to the system. Suppose that the input of DL $v(k)$, output of the system $y_p(k)$ and variation of the input $v(k)$ have the constrains as follows[4]:

$$v_{min} \leq v(k+j) \leq v_{max} \quad (28)$$

$$y_{min} \leq y_p(k+j) \leq y_{max} \quad (29)$$

$$\Delta v_{min} \leq \Delta v \leq \Delta v_{max} \quad (30)$$

Let $\boldsymbol{\alpha} = [1, 1, \cdots, 1]'_{m\times1}, \boldsymbol{\beta} = [1, 1, \cdots, 1]'_{p\times1}$ and $\boldsymbol{R} = [\begin{smallmatrix}1 & 0\\ 1 & 1\end{smallmatrix}]$. Using equation (20) and (27), the vector form of input $\boldsymbol{v}$ can be written as follows:

$$\boldsymbol{v} = v(k-1)\boldsymbol{\alpha} + \boldsymbol{R}\Delta\boldsymbol{v} \tag{31}$$

where, $\boldsymbol{v} = [v(k), v(k+1), \cdots, v(k+m-1)]^T$.
and, using equation (29), vector form of the output $\boldsymbol{y}_p$ can be written as follows:

$$y_{min}\boldsymbol{\beta} \leq \boldsymbol{y}_p \leq y_{max}\boldsymbol{\beta} \tag{32}$$

Then, using equation (28) and equation (31), $v(k)$ can be displayed with $\Delta\boldsymbol{v}$ as follows:

$$\begin{aligned} \boldsymbol{R}\Delta V &\leq (v_{max} - v(k-1))\,\boldsymbol{\alpha} \\ -\boldsymbol{R}\Delta V &\leq (v(k-1) - v_{min})\,\boldsymbol{\alpha} \end{aligned} \tag{33}$$

Using equation (17), equation (29) and equation(32), $y(k)$ can be displayed with $\Delta\boldsymbol{v}$ as follows:

$$\begin{aligned} \boldsymbol{G}\Delta\boldsymbol{v} &\leq y_{max}\boldsymbol{\beta} - [\boldsymbol{F}\boldsymbol{y}_m + H\Delta v(k-1)] \\ -\boldsymbol{G}\Delta\boldsymbol{v} &\leq [\boldsymbol{F}\boldsymbol{y}_m + \boldsymbol{H}\Delta v(k-1)] - y_{min}\boldsymbol{\beta} \end{aligned} \tag{34}$$

Equation (30) can be rewritten as follows:

$$\boldsymbol{R}\Delta v_{min} \leq \Delta\boldsymbol{v} \leq \boldsymbol{R}\Delta v_{max} \tag{35}$$

In summary, using quadratic programming, the optimal variation of input ΔV, can be obtained from the following equations:

$$J = E\{(\boldsymbol{y}_F - \boldsymbol{y}_r)^T(\boldsymbol{y}_F - \boldsymbol{y}_r) + \lambda\Delta\boldsymbol{v}^T\Delta\boldsymbol{v}\} \tag{36}$$

$$s.t. \begin{cases} \boldsymbol{G}\Delta\boldsymbol{v} \leq y_{max}\boldsymbol{\beta} - [\boldsymbol{F}\boldsymbol{y}_m + \boldsymbol{H}\Delta v(k-1)] \\ -\boldsymbol{G}\Delta\boldsymbol{v} \leq [\boldsymbol{F}\boldsymbol{y}_m + \boldsymbol{H}\Delta v(k-1)] - y_{min}\boldsymbol{\beta} \\ \boldsymbol{R}\Delta\boldsymbol{v} \leq (v_{max} - v(k-1))\,\boldsymbol{\alpha} \\ -\boldsymbol{R}\Delta\boldsymbol{v} \leq (v(k-1) - v_{min})\,\boldsymbol{\alpha} \\ \boldsymbol{R}\Delta v_{min} \leq \Delta\boldsymbol{v} \leq \boldsymbol{R}\Delta v_{max} \end{cases}$$

$v(k)$ can be calculated by using equation (27), and using the inverse equation of static nonlinear part of Hammerstein model (equation (5)$\sim$ equation(7)), then, the optimal input $u(k)$ can be calculated with constraints as shown in Fig.3.

4. SIMULATION RESULTS AND DISCUSSIONS

For proving the effectiveness of the proposed algorithm, two simulations have been done for the proposed controller.
In the first simulation, the step type tracking characteristic with the disturbance of the added substrate is demonstrated. The numerical values used for this simulation are given in Table 1 and Table 2. The simulation results are shown from Fig.5 to Fig.9. The disturbance is an acid stream $q1$. $q1$ is changed from 15.75ml/s to 17ml/s as shown in Fig.5. Fig.6 displays the plant output with a dotted line, reference set-point with a continuous line and model output with a dashed line. It shows that the outputs of plant and model are converged to reference set-point after 500 sampling times. Fig.7 displays the control input $q3$. It also converged to about $15ml/s$ when $t \rightarrow \infty$. Fig.8 displays the error between the output of plant and the referential set-point. The error is converged to zero when $t \rightarrow \infty$. Excellent tracking characteristic is shown by using the presented controller. Fig.9 displays the error between the plant and the identified model. The error is converged to zero when $t \rightarrow \infty$. It is proved that the identified model is matched to the plant. From Fig.5 to Fig.9, they show that the proposed controller has good performance to the disturbance.
In the second simulation, the presented controller ANCMPC and Adaptive Nonlinear Model Predictive Control (ANMPC) are compared in variable set-point condition. The numerical values used for this simulation are given in Table 1 and Table 2. Fig.10 displays the plant outputs by using the controller ANMPC (dashed line), the plant output by using the controller ANCMPC (continuous line), and the reference line (dotted line). It shows that the tracking performance of the proposed controller is better than that of the controller ANMPC. Fig.11 displays the control input value $q3$ by using ANMPC. The control input $q3$ has two overshoots when the reference set-point changes from 6.5 to 7 and from 7 to 7.5. The values of overshoot is over 400 ml/s. Fig.12 displays the control input value $q3$ by using ANCMPC. The input for ANCMPC is compared with that for ANMPC. It shows that the overshoot in ANCMPC is smaller than that in ANMPC. It is proved that the input performance of the proposed controller is better than that of the controller ANMPC for variable set-point condition after using constraints. Fig.13 displays the error between the plant and the model using ANMPC (dashed line) and ANCMPC (continuous line). It is proved that the matching performance of the proposed controller is better than that of controller ANMPC. As the simulation results, the proposed controller has good tracking performance under the disturbance, the noise and the variable reference set point.

5. CONCLUSION

In this paper, an adaptive nonlinear constrained model predictive control is proposed. Simulation results show that the proposed controller has good control tracking performance to the varying substrate feeding disturbance. The proposed controller is compared with adaptive nonlinear model predictive control without constraints. Simulation results show that the input characteristic of ANCMPC is more better than that of ANMPC after using the constraints. The variable set-point tracking performance of the proposed controller is also better than that of the controller ANMPC.

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Table 1. The numerical values for simulation

Symbol	Value/unit
A	$200cm^2$
h	125.0 mm
W_{a_1}	$3\times10^{-3}/mol \cdot L^{-1}$
W_{a_2}	$-3\times10^{-2}/mol \cdot L^{-1}$
W_{a3}	$-3.06\times10^{-3}/mol \cdot L^{-1}$
W_{b_1}	0
W_{b_2}	$3\times10^{-2}/mol \cdot L^{-1}$
W_{b3}	$5.00\times10^{-5}/mol \cdot L^{-1}$
pK1	6.35
pK2	10.2503
dt	5s
p	10
m	3

Table 2. The Initial values for simulation 1 and 2

Symbol	Value/unit
q_1	15.75 (ml $\cdot s^{-1}$)
q_2	0.55 (ml $\cdot s^{-1}$)
q_3	13.1 (ml $\cdot s^{-1}$)
W_{a4}	$-4.50\times10^{-4}/mol \cdot L^{-1}$
W_{b4}	$-4.50\times10^{-4}/mol \cdot L^{-1}$
pH4	7.00

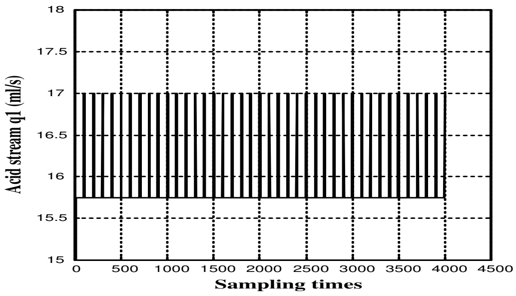

Fig. 5. The Acid stream $q1$ by using ANCMPC

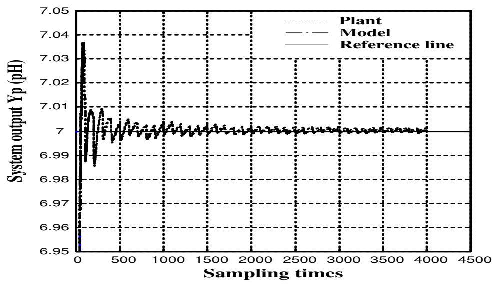

Fig. 6. The output value of the plant and the model by using ANCMPC

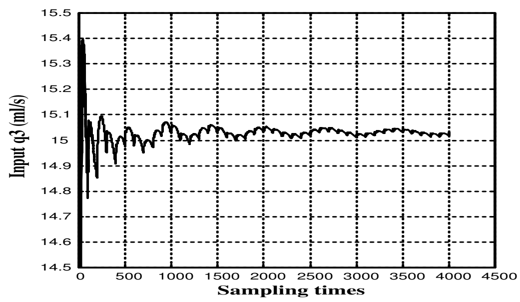

Fig. 7. The input value $q3$ by using ANCMPC

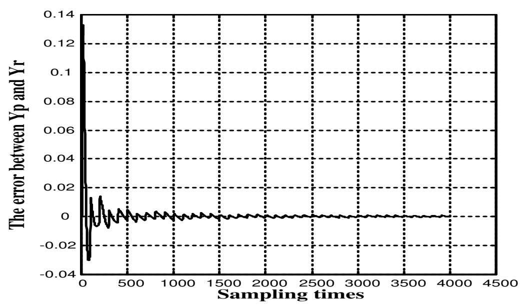

Fig. 8. The output error between the plant and the reference by using ANCMPC

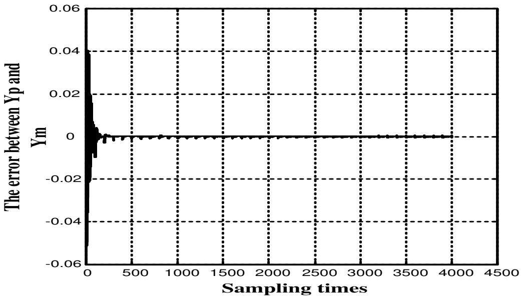

Fig. 9. The output error between the plant and model by using ANCMPC

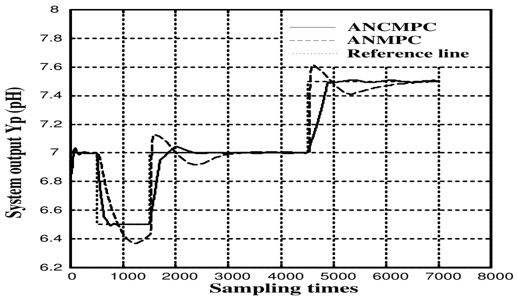

Fig. 10. The output Yp (pH) by using ANMPC and ANCMPC

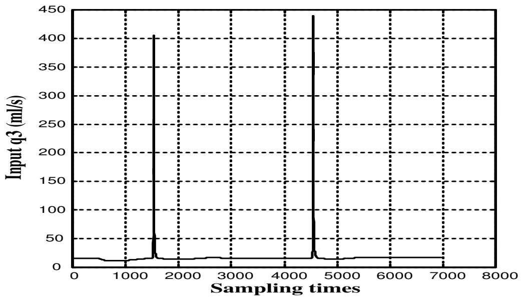

Fig. 11. The input value $q3$ by using ANMPC

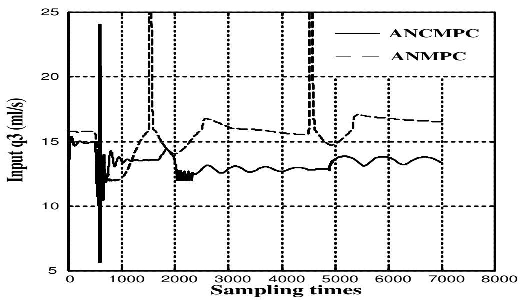

Fig. 12. The input value $q3$ by using ANCMPC

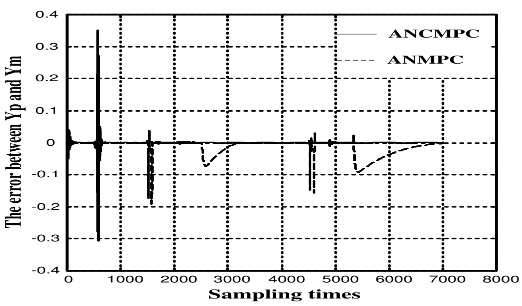

Fig. 13. Error between y_p and y_m