Adaptive Control of pH Neutralization Process based on Feedback Linearization Technique

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Abstract. This paper presents a nonlinear adaptive controller for pH neutralization process, which is difficult to control due to its nonlinear dynamics, sensibility to small disturbance and time-varying characteristics. Special attention is paid to the effect of internal perturbations and external disturbances typically present in the chemical process. In this work, the performance of the adaptive nonlinear controller based on feedback linearization (FL) is compared with the performance of a conventional PID controller for pH control. It is shown that conventional PID controller rejects input disturbances with poor performance, and the proposed control technique can reject the input disturbances from the control signal and then recovers linear reference tracking very well.

1. Introduction
The control of pH is common in the chemical process and biotechnological industries. For instance, the pH of effluent streams from wastewater treatment plants must be maintained within stringent environmental limits [1], [2]. Tight control of pH is also critical in the production of pharmaceuticals [3]. However, high performance and robust pH control are often difficult to achieve due to nonlinear and time-varying process characteristics. These processes can exhibit severe static nonlinear behavior because the process gain can vary several orders of magnitude over a modest range of pH values. Moreover, the titration curve may be time-varying due to unmeasured changes in the buffering capacity. So far, many authors have proposed nonlinear control strategies to overcome the difficulties that evolved in pH control. It must be noted that pH neutralization process is widely studied for two different reasons. First, because of its environmental effects, especially when effluent or wastewater has to be neutralized before being discharged into the environment. Second, pH neutralization process is highly nonlinear and is known as a challenging problem. As a result of these characteristics, several adaptive nonlinear control strategies [4]-[9] have been proposed for pH neutralization processes. Gustafsson and Waller [10] designed a nonlinear adaptive controller. Through a simulation study, they found that the proposed nonlinear adaptive controller outperforms those of the conventional proportional integral differential (PID) and linear adaptive controllers. Wright et al. [11] introduced an online identification algorithm for unknown chemical species in the estimation of the strong acid equivalent and constructed a nonlinear adaptive controller. Lakshmi et al. [12] proposed an adaptive internal model control technique which is based on the concepts of nonlinear internal model control, strong acid equivalent, and a simplified adaptive mechanism. Although the techniques showed satisfactory performance in the exemplary pH process model, it may not work properly for more complex neutralization processes when there is a change in the buffering solution due to the use of
strong acid equivalent and simple adaptation mechanism. Among different nonlinear control techniques, feedback linearization (FL) [13-15] algorithm has attracted researchers’ attention. Feedback linearization is linearizing a nonlinear system by cancelling its nonlinearities in order to apply abundant linear control theories to the linearized system. Adaptive nonlinear control schemes can be designed by combining such nonlinear controllers mentioned above with parameter estimation algorithms in a variety of ways. In this paper, it is shown that the proposed method gives a good response for both set point tracking and disturbance rejection performance.

The rest of the paper is organized as follows. Section 2 presented the modeling of the pH. In Section 3, the parameter estimator and the feedback linearized controller is applied to a pH process and identity of this scheme has been shown. Section 4 presents the stability analysis of the parameter estimator. Simulation results are shown in Section 5. Finally, Section 6 presents the conclusion.

2. The Reaction Invariant Model

A simplified schematic diagram of the pH neutralization process is shown in Fig. 1. The process consists of an acid stream (q1), buffer stream (q2) and the base stream (q3) that is mixed in tank 1. The output of the process is the pH value of the effluent stream (pH4), and the flow rate of the titrating stream (q3) is the control input. A dynamic model is derived using the conservation equations of the reaction invariants and equilibrium relations [16]. The modeling assumptions include perfect mixing, a constant volume of the tank (V), constant density, and complete solubility of the ions involved. The chemical reactions that occurred in the system are:

\[ \text{H}_2\text{CO}_3 \leftrightarrow \text{HCO}_3^- + \text{H}^+ \]
\[ \text{HCO}_3^- \leftrightarrow \text{CO}_3^{2-} + \text{H}^+ \]
\[ \text{H}_2\text{O} \leftrightarrow \text{OH}^- + \text{H}^+ \]

The equilibrium constants for the reaction are:

\[ K_{a1} = \frac{[\text{HCO}_3^-][\text{H}^+]}{[\text{H}_2\text{CO}_3]} \]
\[ K_{a2} = \frac{[\text{CO}_3^{2-}][\text{H}^+]}{[\text{HCO}_3^-]} \]
\[ K_w = [\text{H}^+][\text{OH}^-] \]
The chemical equilibria are modeled using the reaction invariant concept [17]. For this system, concentrations of reaction invariants are defined for each stream \((i=1,2,3,4)\):

\[ W_{ai} = [H^+]_i - [OH^-]_i + [HCO_3^-]_i - 2[CO_3^{2-}]_i \]

\[ W_{bi} = [H_2CO_3]_i + [HCO_3^-]_i + [CO_3^{2-}]_i \]

where \(W_{ai}\) is a charge-related quantity, while \(W_{bi}\) represents the concentration of the carbonate ion. These are independent of the extent of the reaction. The hydrogen ion concentration can be determined from \(W_{ai}\) and \(W_{bi}\):

\[ \frac{W_{bi} K_{a1} [H^+]_i + 2K_{a1}K_{a2} [H^+]_i^2 + W_{ai} + K_w}{1 + K_{a1} [H^+]_i + K_{a1}K_{a2} [H^+]_i} - [H^+]_i = 0 \]

The pH for the effluent stream is calculated by the following relationship with the hydrogen ion \([H^+]_4\):

\[ [H^+]_4 pH_4 = -\log_{10}([H^+]_4) \]

A dynamic model of the effluent stream is obtained by the material balance of a vessel as follows:

\[ V \frac{dW_{a4}}{dt} = q_1 (W_{a1} - W_{a4}) + q_2 (W_{a2} - W_{a4}) + q_3 (W_{a3} - W_{a4}) \]

\[ V \frac{dW_{b4}}{dt} = q_1 (W_{b1} - W_{b4}) + q_2 (W_{b2} - W_{b4}) + q_3 (W_{b3} - W_{b4}) \]

The state-space model of the process is then given by

\[ \dot{x} = f(x) + g(x)u + p(x)d \tag{1} \]

where

\[ x = [W_{a4} W_{b4}]^T, \quad u = q_3, \quad d = [W_{a1} W_{b1}]^T \]

\[ f(x) = \begin{bmatrix} -\frac{q_1}{V}x_1 + \frac{q_2}{V} (W_{a2} - x_1) \\ -\frac{q_1}{V}x_2 + \frac{q_2}{V} (W_{b2} - x_2) \end{bmatrix}, \quad g(x) = \begin{bmatrix} \frac{1}{V} (W_{a3} - x_1) \\ \frac{1}{V} (W_{b3} - x_2) \end{bmatrix}, \quad p = \begin{bmatrix} q_1 \\ 0 \\ 0 \\ q_1 \end{bmatrix}. \]

Note that the vector \(d\) contains the unknown parameters, and "(1)" is linear in \(p\). The nonlinear relation between the output \(y\) and the state variables \(x\) is given by

\[ c(x,y) = 0 \tag{2} \]

where

\[ c_{x_2} = \frac{1 + 2 \times 10^{y-pk_2}}{1 + 10^{pk_1-y} + 10^{y-pk_2}}, \quad c(x,y) = x_1 + 10^{y-14} - 10^{-y} + x_2 c_{x_2} \tag{3} \]
\( p_{k_1} = -\log_{10} k_{a1}, \quad p_{k_2} = -\log_{10} k_{a2}. \)

The nominal values of the parameters are given in Tab I. The open-loop responses in Fig. 2 shows the nonlinear and time-varying characteristics of the model. For constant buffer flow rates of 0.55 and 0 ml/s, the model is subjected to +/- 10% step changes in the base flow rate. When \( q_2 = 0.55 \) ml/s, the steady state gain for the + 10% change is very large than the steady state gain in - 10% change. For the case \( q_2 = 0 \) ml/s, the steady state gain for - 10% is very large than the gain in - 10% when \( q_2 = 0.55 \) ml/s.

![Figure 2. Open-loop responses for +/- 10% step change in base stream.](image)

**Table 1. Nominal Plant Parameters**

| Parameters | Nominal Values |
|------------|----------------|
| \( V \)    | 2900 ml        |
| \( k_{a1} \) | \( 4.47 \times 10^{-7} \) |
| \( k_{a2} \) | \( 5.62 \times 10^{-11} \) |
| \( [q_1] \) | 0.003 M HNO3 |
|           | \( 5 \times 10^{-5} \) M H2CO3 |
| \( [q_3] \) | 0.03 M NaHCO3 |
| \( [q_3] \) | 0.003 M NaOH |
|           | \( 5 \times 10^{-3} \) M NaHCO3 |
| \( q_1 \)  | 16.6 ml/s      |
| \( q_2 \)  | 0.55 ml/s      |
| \( q_3 \)  | 15.8 ml/s      |
| \( \text{pH}_4 \) | 7.00 |
| \( W_{a1} \) | 0.003 M     |
| \( W_{a4} \) | \( 5 \times 10^{-5} \) M |
| \( W_{a2} \) | -0.03 M       |
| \( W_{a4} \) | 0.03 M        |
| \( W_{a3} \) | \(-3.05 \times 10^{-3} \) M |
| \( W_{b3} \) | \( 5 \times 10^{-5} \) M |
| \( W_{b4} \) | \(-4.50 \times 10^{-4} \) M |
| \( W_{b4} \) | \( 5.5 \times 10^{-4} \) M |
3. Adaptive Nonlinear Control Design

The adaptive nonlinear controller proposed in this paper consists of two modules: control and estimation. The two modules are designed separately and then combined using a nonlinear damping term so that the state variables are bounded in the presence of estimation error.

3.1 Estimator Design

A parameter estimator is designed here to satisfy the following requirement:

\[ \tilde{d} := d - \hat{d} \in L_\infty \]  \hspace{1cm} (4)

where \( \hat{d} \) is the estimated value of \( d \). To find an estimator satisfying condition “(4)”, consider the state prediction equation:

\[ \dot{x} = -\eta(x - \hat{x}) + f(x) + g(x)u + p\tilde{d} \]  \hspace{1cm} (5)

where \( \eta \) is stable, and \( N \) is positive definite such that

\[ NN + \eta^T N = -S, \quad S = S^T > 0. \]  \hspace{1cm} (6)

Define the state prediction error as follows:

\[ e_1 = x - \hat{x}. \]  \hspace{1cm} (7)

Using this prediction error, we can derive the estimator:

\[ \dot{\hat{d}} = \Psi p^T N e_1, \quad \Psi = \Psi^T > 0. \]  \hspace{1cm} (8)

This estimator is then guaranteed to satisfy the condition “(4)”, as is shown in the following section.

3.2 Feedback Linearization Controller Design

In this section, a nonlinear controller based on feedback linearization technique is discussed. Then the output feedback controller is combined with a parameter estimator which provides online estimates of the unmeasured reaction invariants in the acid stream.

Consider the nonlinear system described by

\[ \dot{x} = f(x) + g(x)u, \quad y = h(x) \]  \hspace{1cm} (9)

The objective is to find a linear differential relation between the output \( y \) and a new input \( v \). The system has a relative degree \( r \) if

\[ L_g L_f^i = 0, \quad 0 \leq i \leq r - 2 \]  \hspace{1cm} (10)

\[ L_g L_f^{r-1} h(x) \neq 0 \]

where \( Lf \) is the Lie derivative in the direction of \( f \). Assume that the above system is linearizable and has the relative degree of \( r \). The input transformation

\[ u = \frac{v - L_f^r h}{L_g L_f^{r-1} h} \]  \hspace{1cm} (11)
results in a linear relation between \( y \) and \( v \) given by

\[
y^{(r)} = v \tag{12}
\]

For pH process taking the time derivative of “(3)” using “(1)” and rearranging yields

\[
\dot{y} = -c_y^{-1}(x, y)c_x(y)[f(x) + g(x)u + p(x)d] \tag{13}
\]

where

\[
c_x = \frac{\partial c(x, y)}{\partial x} = \left[ 1 + \frac{1 + 2 \times 10^{y-pk_2}}{1 + 10^{pk_1-y} + 10^{y-pk_2}} \right],
\]

\[
c_y = (ln10) \times \left\{ 10^{-14} + 10^{-y} + x_2 \left( \frac{10^{pk_1-y} + 10^{y-pk_2} + 4 \times 10^{pk_1-pk_2}}{1 + 10^{pk_1-y} + 10^{y-pk_2}^2} \right) \right\}.
\]

Because \(-c_y^{-1}(x, y)c_x(y)g(x) \neq 0\) for all \( x \) and \( y \) of interest, the model has relative degree \( r = 1 \) and the linearization relation is

\[
u = \frac{v + c_y^{-1}(x, y)c_x(y)[f(x) + p(x)d]}{-c_y^{-1}(x, y)c_x(y)g(x)}
\]

Now, assume \( v \) is the output of a PID controller in the form

\[
v = k_p e + k_i \int e + y_{sp} \tag{14}
\]

where \( e = y_{sp} - y \)

The adaptive version of the above control law is given as:

\[
u = \frac{v + c_y^{-1}(x, y)c_x(y)[f(x) + p(x)d]}{-c_y^{-1}(x, y)c_x(y)g(x)} \tag{15}
\]

The parameter estimator obtained in the previous subsection is then combined with this controller leading to adaptive nonlinear control. Tab II shows the nonlinear estimator tuning parameters.

| Parameters | Nominal Values |
|------------|----------------|
| \( \eta \) | \( \begin{bmatrix} -0.1 \\ 0 \end{bmatrix} \) |
| \( s \) | \( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) |
| \( \psi \) | \( \begin{bmatrix} 0.0 \\ 0 \end{bmatrix} \) |

4. Stability Analysis

The stability of internal dynamics for this model has been proved by [18]. Next, it will be shown that the estimator error subsystem is asymptotically stable. From equation (7), the derivative of the error is

\[
\dot{e}_1 = \dot{x} - \dot{\hat{x}} \tag{16}
\]
Hence,
\[ \dot{e}_1 = \eta e_1 + pd \tag{17} \]

Consider the following Lyapunov candidate
\[ V_e = e_1^T Ne_1 + \hat{d}^T \psi^{-1} \hat{d} \]

Differentiating this and using "(8)" gives
\[ \dot{V}_e = e_1^T Ne_1 + e_1^T N \hat{e}_1 + (\hat{d}^T \psi^{-1} \hat{d} - \hat{d}^T \psi^{-1} \dot{\hat{d}}) \]
\[ \dot{V}_e = (\eta e_1 + pd)^T Ne_1 + e_1^T P (\eta e_1 + pd) - 2(\hat{d}^T \psi^{-1} \dot{\hat{d}}) \]
\[ \dot{V}_e = -e_1^T Se_1 + 2\hat{d}^T (p^T Ne_1 - \psi^{-1} \dot{\hat{d}}) \]

Hence,
\[ \dot{V}_e = -e_1^T Se_1 \leq 0 \]

This ensures that the estimator error subsystem is asymptotically stable.

5. Simulation Results
The performance of the adaptive feedback linearization controller is compared with the performance of a conventional PID controller, tuned with a proportional gain of 113.6 and an integral gain of 8.7, for disturbance rejection and set-point tracking. The unmeasured variations of feed reaction are depicted in Fig.3 and considered as disturbances applied to the system. Fig.4 shows the disturbance rejection performance of a FL controller and the PID controller. It is shown that the direct FL could not damp the disturbance so the adaptive version is needed. Fig.5-7 shows the performances of the adaptive FLC and the PID controller.

Figure 3. Feed stream concentration.
Figure 4. Disturbance rejection performance of the PID and non-adaptive FL controllers.

Figure 5. Disturbance rejection performance of the PID and adaptive FL controllers.
As can be seen, now the performance of the adaptive FL controller outperforms the PID controller since it rejects quickly the input disturbances at the control signal and then recovers linear reference tracking.

6. Conclusion
In this paper, a direct feedback linearization is first designed to control the pH process, but it could not damp the disturbance very well, so an adaptive version is designed. In the adaptive version, the designed nonlinear controller based on the technique of feedback linearization is combined with a parameter estimator. The performance of this controller was compared to the performance of the PID controller. It is shown that the adaptive version of this controller has a superior performance in set-point tracking and disturbance rejection over the performance of the conventional PID controller.

7. References
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