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pH공정의 적응제어
Adaptive Control for pH Systems

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Abstracts : An Adaptive pH control is developed to manipulate the nonlinearities and time-varying properties of pH systems. In this research, we estimate two adjustable parameters by using the recursive least squares method and a nonlinear PI controller is used to control pH systems based on the estimated two parameters.
Key words: pH process, nonlinearity, adaptive control, estimator

1. Introduction

The control of the pH neutralization process plays a very important role in chemical industries, such as wastewater treatments, polymerization reactions, fatty acid production, biochemical processes, and so on. The pH neutralization process shows a strong nonlinear behavior and time-varying nonlinear characteristics resulted from the variation of the feed components or total ion concentrations. These behaviors cause many difficulties in controlling the pH process with conventional control technique such as the PID controller. Thus, many researchers have exerted much of their effort in the modeling and control study of pH processes.

McAvoy et al. (1972) modeled the pH process with the material balance and equilibrium equations. Gustafsson and Waller (1983) introduced the concept of reaction invariant to incorporate the nonlinearity and designed an adaptive pH control system which has the total ion concentrations of fictitious weak acids as adjustable parameters. Gustafsson (1985) reported the experiment results of the adaptive nonlinear pH controller using reaction invariant concept. Gustafsson and Waller (1992) discussed the relative merits of linear and nonlinear continuous control of pH processes via simulations and experiments. The nonlinear adaptive control strategy can incorporate effectively the time-varying properties and the nonlinearities of the pH process. However, it requires a prior information on the feed stream since the dissociation constants of the fictitious weak acids should be set. Elsewhere, many adjustable parameters are required to represent the pH process including wide variation of dissociation constants.

Williams et al. (1990) developed a two-parameter model which consists of the total ion concentration and dissociation constant of a single fictitious weak acid and designed a controller to control the multi-component pH system where they estimated two parameters by injecting a strong base at two points of in-line neutralization process. However, the method can't be applied to the usual pH process composed of a single pH sensor and a single Continuous-Stirred-Tank-Reactor (CSTR). The model can well approximate the operating region of the pH process and only operating region is important to the controller so that the two-parameter model can produce an almost same control performance as the full-order model (Sung et al. (1995)). For the case of the adaptive control, the on-line recursive estimator for the two-parameter model would show the good robustness to a poorly perturbed pH process and fast adaptation because only two parameters should be estimated by the recursive estimator.

Wright and Kravaris (1991) suggested a first order state equation by reducing reaction invariant pH process models. They proved that the state/output map is a type of the titration curve of the feed stream and the pH process can be completely represented by a first order state equation and the titration curve if the initial state is steady state and the feed composition does not change. They used a PI controller of which the controlled variable is a scaled total ion concentration of the component in the titrating stream (state variable) instead of the measured pH value. Wright et al.(1991) also demonstrated the good control performance and robustness of their control strategy with experimental study. However, good control performance of their strategy can't be guaranteed if the pH process has severe time-varying nonlinear properties.

Lee et al. (1994) proposed a nonlinear self-tuning regulator using the two-parameter model to control the pH process. They estimated the unknown parameters, the concentration and the dissociation constant of the fictitious weak acid by using a recursive least squares method with a variable forgetting factor. The regulator shows a good control performance for multicomponent systems. However, if the sampling time to the time constant of the pH process is relatively large, the good control performance may be degraded because they used the Euler integration method to estimate the derivative of the pH value.

Sung and Lee (1995) improved Lee et al.'s (1993) method by combining Yuwana and Seborg's (1982) PID autotuning strategy with Wright and Kravaris' (1991) pH control strategy. However, in this strategy, the continuous on-line identification is impossible and if disturbances enter during the identification work the identified model is unacceptable. Sung et al (1995) obtained the titration curve of the pH process using an identification reactor, and then controlled the pH process by using Wright and Kravaris' (1991) control strategy. Their identification strategy can incorporate the entire operating region and time-varying properties of the pH process. However, a separated identification reactor and another pH sensor are needed and the identified model contaminated by disturbances is useless.

We propose a new adaptive controller to incorporate the nonlinearities and the time-varying properties of the pH process. It doesn't need any information on the feed composition and adjustable parameters are only two. We estimate the total ion concentration and the dissociation constant of a fictitious weak acid via a recursive least squares method to represent the pH process. A small perturbation signal is systematically added to the controller output to prevent the estimation windup (major difficulty in the practical implementation of the on-line recursive estimator). The proposed control strategy shows good robustness to the measurement noise, various forgetting factors, modeling errors.

2. Modeling of the pH process

Consider a continuous stirred tank neutralization reactor system as in Figure 1 and assume that the feed stream is composed of a single 1-protic weak acid and titrated by a strong base. Then the follwing material balance equations and equilibrium equation can be obtained. Here, the input time delay term can be used to approximate the dynamics of the pH sensor and nonideal mixing.

$$V\frac{dC_a(t)}{dt} = FC_{a0} - (F + u(t-\theta))C_a(t) \quad (1)$$

$$V\frac{dC_b(t)}{dt} = u(t-\theta)C_{b0} - (F + u(t-\theta))C_b(t) \quad (2)$$

$$\frac{K_aC_a}{K_a + \left[\mathrm{H}^+\right]} + \frac{K_w}{\left[\mathrm{H}^+\right]} = \left[\mathrm{H}^+\right] + C_b \quad (3)$$

where,

C_{a0} = total ion concentration of the weak acid in the influent stream

C_a = total ion concentration of the weak acid in the effluent stream

C_{b0} = total ion concentration of the strong base in the titrating stream

C_b = total ion concentration of the strong base in the effluent stream

K_a = dissociation constant of the weak acid

K_w = dissociation constant of water

F = flowrate of the feed stream u = flowrate of the titrating stream

$\left[\mathrm{H}^+\right]$ = hydrogen ion concentration

θ = time delay of the titrating stream

This continuous time system can be transformed to the corresponding discrete time system. We assume that the time delay is smaller than the sampling time for simplicity. However, the following derivations can be easily extended to the case that the time delay is larger than the sampling time. During the future time corresponding to the time delay (θ), C_a and C_b are affected by u_{k-2} and during the remained time to the next sampling ($\Delta t - \theta$), C_a and C_b are affected by u_{k-1}. Therefore, we obtain the following discrete time system.

$$C_{a,k-1,\theta} = C_{a,k-1}E_{k-2} + (1 - E_{k-2})(\frac{FC_{a0}}{F + u_{k-2}}) \quad (4)$$

$$C_{a,k} = C_{a,k-1,\theta}E_{k-1} + (1 - E_{k-1})(\frac{FC_{a0}}{F + u_{k-1}}) \quad (5)$$

$$C_{b,k-1,\theta} = C_{b,k-1}E_{k-2} + (1 - E_{k-2})(\frac{u_{k-2}C_{b0}}{F + u_{k-2}}) \quad (6)$$

$$C_{b,k} = C_{b,k-1,\theta}E_{k-1} + (1 - E_{k-1})(\frac{u_{k-1}C_{b0}}{F + u_{k-1}}) \quad (7)$$

From (4) and (5), we can obtain (8) and (9) can be obtained from (6) and(7)

$$C_{a,k} = C_{a,k-1}E_{k-2}E_{k-1} + E_{k-1}(1 - E_{k-2})(\frac{FC_{a0}}{F + u_{k-2}}) + (1 - E_{k-1})(\frac{FC_{a0}}{F + u_{k-1}}) \quad (8)$$

$$C_{b,k} = C_{b,k-1}E_{k-2}E_{k-1} + E_{k-1}(1 - E_{k-2})(\frac{u_{k-2}C_{b0}}{F + u_{k-2}}) + (1 - E_{k-1})(\frac{u_{k-1}C_{b0}}{F + u_{k-1}}) \quad (9)$$

$$\frac{K_aC_{a,k}}{K_a + \left[\mathrm{H}^+\right]_k} + \frac{K_w}{\left[\mathrm{H}^+\right]_k} = \left[\mathrm{H}^+\right]_k + C_{b,k} \quad (10)$$

$$E_{k-2} = \exp(-\frac{(F + u_{k-2})}{V}\theta) \quad (11)$$

$$E_{k-1} = \exp(-\frac{(F + u_{k-1})}{V}(\Delta t - \theta)) \quad (12)$$

where, subscript k denotes the k-th sampling data and Δt represents the sampling time. Here, with the assumption that F, V, θ and C_{b0} are known, the objective of the on-line estimator is to estimate K_a and C_{a0} to well represent the pH process. This two-parameter model can well approximate the operating region and would provide good robustness and fast adaptation to the recursive on-line estimator because the adjustable parameters are only two.

To estimate the adjustable parameters (K_a and C_{a0}) using a recursive on-line linear estimator, it is necessary to transform the above equations to a linear equation in the adjustable parameters. To do this work, consider the following procedure. First, (10) can be rewritten as follows.

$$K_aC_{a,k} = A_kK_a + A_k\left[\mathrm{H}^+\right]_k \quad (13)$$

$$K_aC_{a,k-1} = A_{k-1}K_a + A_{k-1}\left[\mathrm{H}^+\right]_{k-1} \quad (14)$$

where,

$$A_k = \left[\mathrm{H}^+\right]_k + C_{b,k} - \frac{K_w}{\left[\mathrm{H}^+\right]_k} \quad (15)$$

By inserting (8) into (13), the following equation can be obtained

$$K_aC_{a,k-1}E_{k-2}E_{k-1} + K_aC_{a0}\left\{E_{k-1}(1 - E_{k-2})\frac{F}{F + u_{k-2}} + (1 - E_{k-1})\frac{F}{F + u_{k-1}}\right\} = A_kK_a + A_k\left[\mathrm{H}^+\right]_k \quad (16)$$

where

$$\left[\mathrm{H}^+\right]_k = 10^{-\mathrm{pH}_k} \quad (17)$$

and the following equation is obtained by inserting (14) to (16).

$$K_a\left\{A_{k-1}E_{k-2}E_{k-1} - A_k\right\} + \left\{E_{k-1}(1 - E_{k-2})\frac{F}{F + u_{k-2}} + (1 - E_{k-1})\frac{F}{F + u_{k-1}}\right\}K_aC_{a0} = A_k\left[\mathrm{H}^+\right]_k - A_{k-1}\left[\mathrm{H}^+\right]_{k-1}E_{k-2}E_{k-1} \quad (18)$$

$C_{b,k}$ in (15) can be estimated by (9) and (18) is a linear equation in the adjustable parameters (K_a and C_{a0}). Therefore we can estimate the unknown parameters (K_a and C_{a0}) from (18) using an on-line recursive linear estimator with the forgetting factor. In this study, we would use the recursive least squares method to estimate the unknown parameters (K_a and C_{a0}) from (18).

Here, it should be noted that it is dangerous to continue the parameter adaptation even though the signals (the process output and the controller output) have low support number. That is, the parameter adaptation should be done only when the signals satisfies the persistent excitation condition. Elsewhere, the recursive estimator with the forgetting factor will show a bursting phenomenon (estimation windup) (Anderson (1985)).

The proposed linear equation (18) for the parameter estimation has only two adjustable parameters so that the load of the recursive computation and dangers such as estimation windup and parameters drift phenomenon in the undesired region can much be reduced.

To manipulate the estimation windup phenomenon, several strategies can be used. First, the addition of a small random signal to the controller output can confirm the persistent excitation condition. That is, because all terms of (18) contain the flowrate of the titrating stream (u or controller action), estimation windup problem, the major difficulty in the practical implementation of an on-line recursive estimator can be overcome by adding a small random signal to the controller output. Of course, the signal should be small enough to guarantee negligible fluctuation of the pH value. Second, the identification work can be done only when the process output and input signal are sufficiently rich. Third, a recursive estimator with variable forgetting factor can be used to prevent the bursting phenomenon (estimation windup) (Fortescue et al. (1981), Ydstie et al.

(1985)). Here, we would use the first method because the method is simple and guarantee the persistent excitation condition completely.

Then remaining problem is to determine the magnitude of the random signal. It can be determined as follows using (18). Here, we assume that the time delay is zero because only the controller output difference between the present and the next sampling corresponding to the specified pH value difference is needed.

$$\delta = \left[\min\{|u_{k+1} - u_k|, \delta_{\max}\}\right] random \tag{19}$$

subject to

$$K_a(A_k E_k - A_{k+1}) + K_a C_{a0}(1 - E_k)(\frac{F}{F + u_k}) = A_{k+1}\left[H^+\right]_{k+1} - A_k\left[H^+\right]_k E_k \tag{20}$$

$$K_a(A_{k+1}E_{k+1} - A_{k+2}) + K_a C_{a0}(1 - E_{k+1})(\frac{F}{F + u_{k+1}}) = A_{k+2}\left[H^+\right]_{k+2} - A_{k+1}\left[H^+\right]_{k+1} E_{k+1} \tag{21}$$

$$\left[H^+\right]_{k+1} = 10^{-(pH_k + \alpha)} \tag{22}$$

$$\left[H^+\right]_{k+2} = 10^{-(pH_k + 2\alpha)} \tag{23}$$

$$E_k = \exp(-\frac{(F + u_k)}{V}\Delta t) \tag{24}$$

$$E_{k+1} = \exp(-\frac{(F + u_{k+1})}{V}\Delta t) \tag{25}$$

where, subscript k and *random* denotes the present data and random number between -1.0 and 1.0, respectively and δ denotes the magnitude of the random signal added to the controller output to guarantee the persistent excitation condition. δ_{max} represents the maximum value of the random signal and α is a tuning parameter. By inspection, we can recognize that if the estimated parameters are accurate, (19) confirm that at best, the random signal can change pH value as much as α.

3. Control strategy

We recommend Proportional-Integral (PI) controllers using the titration curve to control the pH process (Wright and Kravaris (1991), Sung and Lee (1995), Sung et al. (1995)). Where, the titration curve is determined by the adjustable parameters (K_a and C_{ao}).

To obtain the titration curve from K_a and C_{ao} estimated by recursive least squares method, consider the following. (1) and (2) can be converted to the following one-dimensional state equation (Wright and Kravaris (1991))

$$V\frac{dx}{dt} + Fx = (1 - x)u \tag{26}$$

$$x = 1 - C_a / C_{a0} = C_b / C_{b0} \tag{27}$$

and then (3) can be rewritten as follows

$$x = \frac{-y^3 - K_a y^2 + (K_w + K_a C_{a0})y + K_a K_w}{C_{b0}y^2 + C_{b0}K_a y + C_{a0}K_a y} = F(pH) \tag{28}$$

where,

$$y = \left[H^+\right] \tag{29}$$

(26) is exact when the composition of the feed stream doesn't change, that is in the steady state and we can recognize that x is a normalized total ion concentration of the strong base in the reactor. Therefore, (28) is another representation of the titration curve.

In this study, the pH control structure of Figure 2 is used to control the pH process. Here, the total ion concentration (C_b) of the strong base in the reactor is continuously estimated by (9) and the adjustable parameters are estimated from (18) by the recursive least squares method with the forgetting factor. Then (28) is used to convert the measured pH value and the set point value to the corresponding scaled total ion concentration x and x_s and then the PI controller would control this x value instead of the pH value. Therefore, roughly speaking, the PI controller would control the material balance system of (26) rather than the nonlinear pH system of (1),(2) and (3). The material balance system (26) is almost linear to the controller output and shows very simple dynamics so that the linear PI controller using the titration curve is sufficient to control the nonlinear pH process (for details, refer to Wright and Kravaris (1991), Sung et al. (1995)).

We developed a predictive control strategy based on the proposed on-line recursive estimator. However, we would not refer to the predictive control strategy because the PI controller is familiar to the field operator and simple and robust to the modeling error. Moreover, the control performance of the predictive control strategy is almost the same as that of the PI controller because the material balance equations of the pH system are very simple and has small time delay term so that high control performances can be achieved by using the PI controller with the titration curve.

4. Practical issues

In the practical implementation of the adaptive pH controller, several issues should be carefully considered. In this section, we would discuss these practical issues.

On-line recursive estimator has several parameters such as the forgetting factor, initial covariance matrix and initial adjustable parameters. We should assign these parameters before implementation. Consider the following recursive least squares method to estimate unknown parameters vector θ in $y(k) = \varphi^T(k)\theta$

$$\theta(k) = \theta(k-1) + K(k)\varepsilon(k) \tag{30}$$

$$\varepsilon(k) = y(k) - \varphi^T(k)\theta(k-1) \tag{31}$$

$$K(k) = P(k)\varphi(k) = P(k-1)\varphi(k)/[\lambda + \varphi^T(k)P(k-1)\varphi(k)] \tag{32}$$

$$P(k) = \{P(k-1) - P(k-1)\varphi(k)\varphi^T(k)P(k-1)/[\lambda + \varphi^T(k)P(k-1)\varphi(k)]\}/\lambda \tag{33}$$

Here, λ and $P(k)$ denote the forgetting factor and the covariance matrix. $\theta(k)$ and $\varphi(k)$ vectors represent unknown parameters and known quantities.

$P(0)$ reflects the confidence in initial estimate $\theta(0)$. That is, if $P(0)$ is small then K(k) will be small and then the estimated parameters θ will not change too much from $\theta(0)$. On the other hand, if $P(0)$ is large, the estimated parameters will quickly jump away from $\theta(0)$. Usually, covariance matrix is initialized by the following equation.

$$P(0) = \rho I \tag{34}$$

Here, I denotes the identity matrix. It can be easily proved that as ρ goes to infinity, the parameter estimate converges to that of the off-line least squares method. Therefore, if we want to neglect the initial parameter estimate, we should choose ρ as a very large value.

The measurements obtained previously are discounted by the forgetting factor λ. Usually, the forgetting factor are chosen as a value between 0.8 and 0.99. The smaller the ρ value, the quicker the information in the previous data will be forgotten and vice verse. In the other hand, too small ρ value will provide an oscillatory parameter estimate when uncertainties such as measurement noises and structural mismatches exit. Contrarily, the robustness to uncertainties can be increased by increasing the forgetting factor (for clarity, refer to the simulation study).

If the signals (controller outputs and process outputs) don't change according to the time, the covariance matrix $P(k)$ goes to infinity. Then the large gain of (32) can produce the burst phenomenon to a small perturbation in $\varepsilon(k)$ such as measurement noises, disturbances. This is called as the estimation windup. In (33), the ρ value is located in the denominator so that the smaller ρ value will cause the estimation windup more frequently. To prevent this phenomenon, many techniques can be used(for detail, refer to the "Modeling of the pH process" section).

Also, the actuator such as valve or pump should be chosen carefully. If the resolution of the actuator is low, the identified model becomes inaccurate as well as the control performance can be very poor. The low resolution actuator such as pneumatic valve without positioner is not recommended to control the process precisely or to obtain the accurate model. Elsewhere, it causes an sustained oscillatory response in the steady state and the obtained model would be unreasonable. Because the low resolution results in severe nonlinearities, it is difficult to inspect the effects of the low resolution using an usual linear model. The following quantizer can be used to simulate the effects of the actuator resolution.

$$u_q(k) = iR \tag{35}$$

$$\text{subject to } iR \le u(k) < (i+1)R \tag{36}$$

$$R = {u_{\max}}/{N} \tag{37}$$

Here, N denotes the actuator resolution to the maximum controller output u_{max}. $u(k)$ and $u_q(k)$ are the controller output and the actuator output (the quantized controller output), respectively. i is an integer value between 0 to N. The effect of the quantization in the pH process will be referred to in the simulation study.

5. Simulation study and discussions

We considered the following pH process to show the control performance and robustness of the proposed control strategy to measurement noises, modeling errors. Here, the first feed stream is composed of 0.01 mol/l HCL and 0.02mol/l H_3PO_4 and are replaced by the second feed stream composed of 0.01 mo/l HCL, 0.02mol/l H_3PO_4 and 0.02 mol/l CH_3COOH at 1500sec and at 2500sec, it is replaced by the third feed stream composed of 0.01 mol/l HCL and 0.02 mol/l CH_3COOH. The random signal corresponding to $\alpha = 0.03$ is added to the controller output to guarantee the persistent excitation condition.

Also, we simulated the effects of the choice of the parameters in the recursive least squares method. Additionally, the effects of the quantization to the parameter estimation and control performance are simulated.

From the simulation results, we can recognize that the proposed control strategy provides good control performances without any information on the feed composition. It shows good robustness to measurement noises and the modeling errors in the material balance equation. Through several simulations, we inspected the effects of several parameters in the on-line recursive estimator to suggest the guidelines in choosing the parameters.

6. Conclusions

Adaptive controller using the titration curve updated by on-line recursive least squares method is proposed to incorporate the nonlinearities and time-varying characteristics of the pH process. Also, we discussed several practical issues associated with the implementation of the adaptive pH controller. The proposed method shows a good control performance and robustness to various measurement noises and modeling errors. It doesn't need a prior information on the feed composition. The addition of the small random signal to the controller output can guarantee the persistent excitation condition. In the future work, we would experimentally verify the performances of the proposed control strategy in neutralization processes of multicomponent influent streams.

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