Comparison of Linear and Nonlinear Adaptive Control of a pH-Process

Grazyna A. Pajunen

ABSTRACT: Physical inspection leads to the modeling of a pH-reactor by a linear dynamic flow and mixing process followed by a static nonlinearity. In this paper, a pH process very difficult to control is simulated for testing different types of adaptive algorithms. In one scheme, the flow and mixing model is assumed to be known. The nonlinear adaptive controller is constructed based on a combination of a pole-placement design method with a piecewise-polynomial approximation of a titration function, the coefficients of which are estimated from pH measurements. In another scheme, an inverse overall process model is obtained by the combination of the flow and mixing model with a piecewise-polynomial approximation of the titration curve. This model is applied to the development of a nonlinear controller based on the model reference adaptive technique. Both methods are applied for tracking a given pH-variable and for regulation. The effectiveness of linear and nonlinear adaptive controllers, obtained using the linear or nonlinear approximation of the titration curve, respectively, is examined and compared for different process solutions and different applications.

Introduction

The pH of a process is defined as the logarithm to the base 10 of the reciprocal of the hydrogen ion activity in a solution. For dilute solutions, as considered here, it is possible, with good accuracy, to use the hydrogen ion concentration instead of activity. The scale is adjusted so that pH equal 7 means the acidic H^+ and basic OH^- radicals are equal. The main difficulty with controlling pH-processes in continuous stirred tank reactors arises from the nonlinear dependence of the pH-value on the amount of reagent (the so-called titration function). If this nonlinearity is severe and changes widely in an unpredictable way, classical linear feedback does not always achieve satisfactory performance [1]–[3]. One possible solution is to apply an adaptive controller, such as a self-tuning proportional-integral-derivative (PID) controller, a minimum-prediction error adaptive controller, or an adaptive controller for closed-loop pole assignment based on an approximate linear process model [4]–[7].

However, since the pH-process is usually dominated by nonlinear characteristics, it could be advantageous to use a nonlinear model rather than an approximate linear model. The usefulness of the nonlinear model depends on how well the structure of the model matches the characteristics of the process. In the cases when only strong (fully dissociated) components are present in the solution (theoretical case), or when the dissociation constants of weak components are known a priori, it is possible to develop a nonlinear process model, based on physicochemical rules, which agree exactly with the real process. Nonlinear adaptive controllers based on these process models give superior performance to either the classical controller or the linear adaptive controller [8], [9].

In this work, the problem considered involves adaptive control of a general pH-process with unknown and time-variant composition. The main goals are to compare the effectiveness of the controllers and to give limitations of adaptive controllers based on linear and nonlinear input-output modeling of the process. The components of the process solutions are chosen so that the titration curves are very nonlinear, and change in shape drastically with the concentrations. The process gain at pH equal 7 for solutions considered in the paper varies by a factor of 50, depending on the concentrations. Compensation for flow changes is also included.

Specification and Model of Process

The processes that determine the output pH of a continuous-flow vessel can be considered to consist of two parts (Fig. 1). A linear dynamic model describes the transport of the liquid elements, such as strong acids A, strong bases B, weak acids α, and weak bases β, from input to output. This is followed by a static nonlinearity, which describes the reversible equilibrium of the chemicals at the output [10]. A flow model consisting of a perfect mixer in series with a plug flow element is often used to describe relatively well-mixed vessels, such as the one considered here. Thus, the following equations are obtained for the concentrations [11]:

$$V\dot{C}_{\alpha\beta} = FC_{\alpha\beta P}(t - t_d) - (F + F_r)\, C_{\alpha\beta}(t) \quad (1)$$

$$V(\dot{C}_A - \dot{C}_B) = F/(C_A - C_B)_P(t - t_d) - (F + F_r) \times (C_A - C_B)(t) \quad (2)$$

$$V\dot{C}_r = F_r C_{rc}(t - t_d) - (F + F_r)\, C_r(t) \quad (3)$$

$$t_d = V_d/(F + F_r)$$

Here F is the process flow; F_r the reagent flow; V the perfectly mixed partial volume; V_d the partial volume of the plug element; C_{rc} the concentration of the reagent stock; C_r the reagent concentration at the reactor output; and $C_{\alpha\beta P}$ and $(C_A - C_B)_P$, and $C_{\alpha\beta}$ and $(C_A - C_B)$ are, respectively, process concentrations at the input and output points of the reactor.

If the time t_d is much less than the sampling interval (T), the discrete-time process model corresponding to Eq. (3) with F_r much less than F is

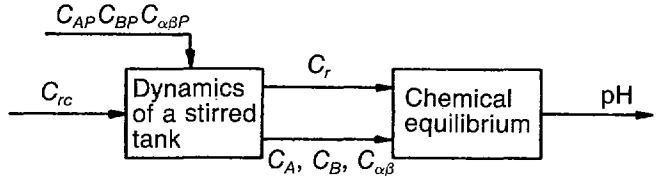


Fig. 1. Model of a pH reactor.

Presented at the 1985 Conference on Decision and Control, Fort Lauderdale, Florida, December 11-13, 1985. Grazyna A. Pajunen is an Assistant Professor in the Department of Electrical and Computer Engineering, Florida Atlantic University, Boca Raton, FL 33431.

0272-1708/87/0200-0039 $01.00 © 1987 IEEE

$$C_r(t) = a_1 C_r(t-1) + b_0 C_{rc}(t-1) + b_1 C_{rc}(t-2) \quad (4)$$

where

$$a_1 = \exp(-T_1)$$

$$b_0 = [1 - \exp(-m_1 T_1)]\, F_r/F$$

$$b_1 = [\exp(-m_1 T_1) - \exp(-T_1)]\, F_r/F$$

$$m_1 = 1 - t_d/T$$

$$T_1 = FT/V$$

Here the titration function (or, more exactly, its inverse) is approximated by the piecewise-polynomial function as follows: where m is the number of intervals, pH_0, pH_1, ..., pH_m are the breakpoints; n is the polynomial order; and γ_{ji} the constant coefficients.

$$C_r(t) = \sum_{j=1}^{m} \psi_j \left\{ \sum_{i=1}^{n} \gamma_{ji} pH(t)^i \right\}$$

$$\psi_j = 1, \quad \text{for } pH_{j-1} \le pH(t) < pH_j \quad (5)$$

$$= 0, \quad \text{otherwise}$$

The number of intervals, the breakpoints, and the polynomial order must be chosen a priori so the nonlinearity and its approximating curve are as close as possible while using the minimum number of parameters. Here the approximation was done by trial and error; however, more sophisticated algorithms could be developed to obtain this match automatically. When the nonlinearity is changing widely in an unpredictable way, it might be more suitable to use an approximate linear model rather than the nonlinear one, as shown below, based on several simulation test results. The coefficients γ_{ji} should be matched to the particular titration curve. Using Eqs. (4) and (5), the inverse of the combined input-output process model is obtained as

$$C_{rc}(t-1) = -b_1 C_{rc}(t-2) + \sum_{j=1}^{m} \psi_j \left\{ \sum_{i=1}^{n} [\beta_{ji0} pH(t) - \beta_{ji1} pH(t-1)^i] \right\} \quad (6)$$

where $\beta_{jir} = a_r \gamma_{ji}$ for all

$i = 1, 2, \ldots, n$; $j = 1, 2, \ldots, m$;

$r = 0, 1$; and $a_0 = 1$

Since the steady-state gain of the linear and nonlinear parts cannot be separated, the combined model will contain one arbitrary constant, so the parameter b_0 has been set equal to 1 in Eq. (6). The inverse of the combined process model is linear in the parameters.

The advantage of this representation in pH-process control is that the components of the process solution do not need to be known. On the other hand, a clear disadvantage is that if this knowledge is available, it cannot be directly incorporated.

The following data were used for process simulation: tank volume, 3 liters; process time delay, 10 sec: and main flow through the system, 1 liter/min. The process solutions are chosen so that the considered pH-process is extremely difficult to control. All solutions consisted of the same chemical compounds, but the concentrations and ratios of these chemicals varied from solution to solution, as shown in the Table.

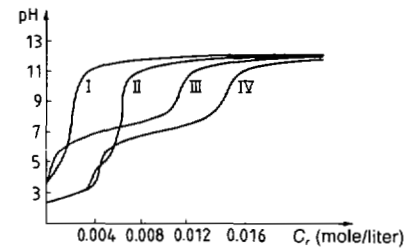
The calculated titration curves of the considered solutions are shown in Fig. 2. Concentration disturbances in the process occur when the process flow changes from one solution to another.

Controller Design for Known Process Parameters

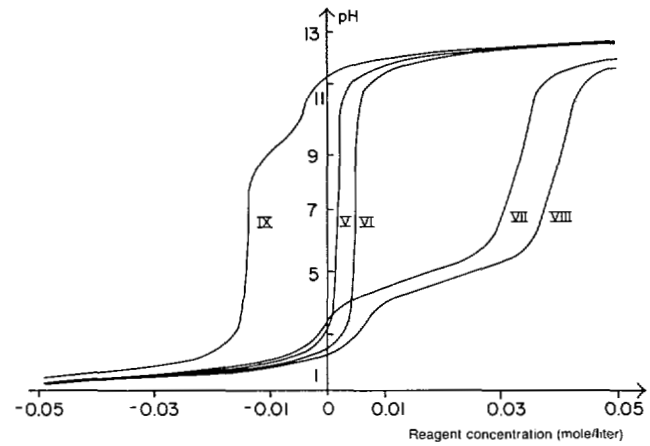
In order to design the controller, an implicit reference model strategy is used. The design procedure includes two steps: predictor design and control computation. This method has been described by Landau [12] for a linear process model.

Table
Concentrations of Species in Process Feed Stocks

	Concentrations (mole/liter)10^{-3}								
Components	**I**	**II**	**III**	**IV**	**V**	**VI**	**VII**	**VIII**	**IX**
HCl	2.5	6.5	1.5	6.5	1	4	2	9	0
NaOH	0	0	0	0	0	0	0	0	5
4-nitrophenol	0.2	0.2	10	10	0	0	3	3	0.2
Pyridine	2	2	0.5	0.5	0	0	0	0	0
Ammonia	0.35	0.35	0.5	0.5	0.35	0.35	3	3	10
Ethanoic acid	0	0	0	0	1	1	30	30	1



(a)



(b)

Fig. 2. Calculated titration curves of process feed stocks.

The predictor for the linear system given by Eq. (4) is given as

$$\hat{C}_r(t+1) = a_1 C_r(t) + b_0 C_{rc}(t) + b_1 C_{rc}(t-1) \quad (7)$$

Using Eq. (5) in Eq. (7) yields

$$\sum_{j=1}^{m} \psi_j \sum_{i=1}^{n} \gamma_{ji} \mathrm{p\hat{H}}(t+1)^i = \sum_{j=1}^{m} \psi_j \sum_{i=1}^{n} s_{ji}^* \mathrm{pH}(t)^i + b_0 C_{rc}(t) + b_1 C_{rc}(t-1) \quad (8)$$

where $s_{ji}^* = \gamma_{ji} a_1$ for all

$$i = 1, 2, \ldots, n;$$
$$j = 1, 2, \ldots, m$$

The control signal is computed so that

$$\mathrm{p\hat{H}}(t+1) = y_M(t+1) \quad (9)$$

where $y_M(\cdot)$ is the output of the reference model, which specifies the desired objectives given by the user. In the present case, the reference model has been chosen as follows:

$$y_M(t) = (1-\kappa) q^{-1} (1-\kappa q^{-1})^{-1} \mathrm{pH}_r(t) \quad (10)$$

where κ is defined as $\exp(-T/\tau)$, τ is the time constant of the desired closed-loop transfer function, pH_r is the reference signal, and q^{-1} is a unit delay operator.

Using Eqs. (8) and (9) and recalculating, the following control law is obtained:

$$C_{rc}(t) = \sum_{j=1}^{m} \psi_j \boldsymbol{\theta}_j^T \boldsymbol{\phi}_1(t) \quad (11)$$

where

$$\boldsymbol{\theta}_j^T = [\gamma_{j1} \ldots \gamma_{jn}\ s_{j1}^* \ldots s_{jn}^* b_1]$$

$$\boldsymbol{\phi}_1^T(t) = [y_M(t+1)^1 \ldots y_M(t+1)^n - \mathrm{pH}(t)^1 \ldots - \mathrm{pH}(t)^n - C_{rc}(t-1)]$$

Adaptive Control Schemes

Since the flow and mixing model as well as the titration curve are considered as unknown constant or time variant, the paramters in control law (11) are also unknown constants or time variant. Two different adaptive schemes are considered. In the first scheme, all parameters in control law (11) are estimated in the closed loop. The series model reference adaptive system (MRAS) structure is proposed here in order to obtain the adjustable system, which is linear in its parameters, as shown in Fig. 3. In the second scheme, the parameters of the dynamic part of the model in Eq. (4) are assumed to be initially known and, since they are directly related to the flow through the reactor, their adaptation is open loop based on the flow measurements. This open-loop adaptation is combined with the closed-loop adaptation of the coefficients γ_{ji} in the static nonlinearity approximation given by Eq. (5), as shown in Fig. 4.

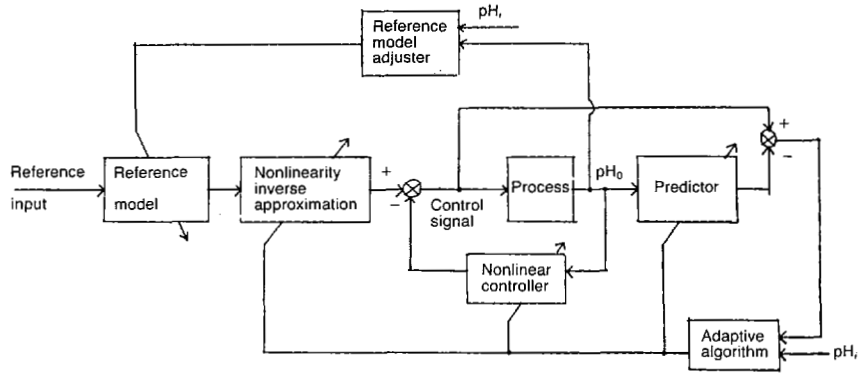


Fig. 3. Adaptive control scheme using implicit model reference strategy.

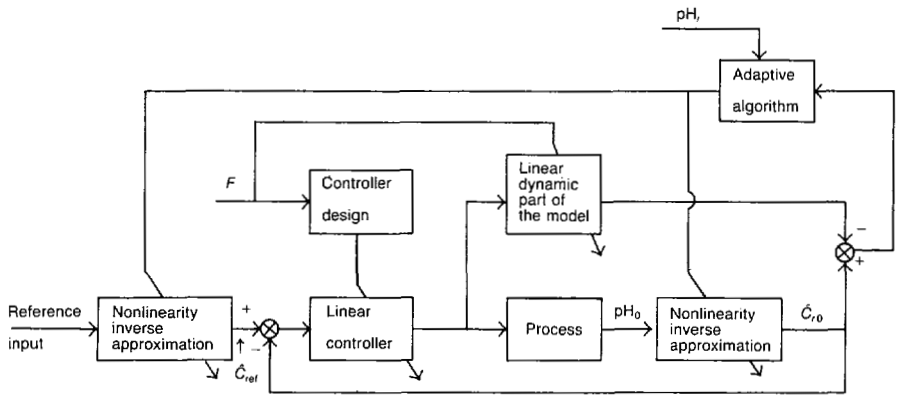


Fig. 4. Self-tuning controller using feedforward adaptation of the linear part of the model based on flow measurement.

First Scheme

The first scheme is based on the model in Fig. 3. Rearranging Eq. (8) and substituting the unknown parameters with their estimates, an adaptive predictor can be written as follows:

$$\hat{C}_{rc}(t) = \sum_{j=1}^{m} \psi_j \hat{\boldsymbol{\theta}}^T(t)\, \boldsymbol{\phi}(t-1) \quad (12)$$

where

$$\boldsymbol{\phi}^T(t) = [\mathrm{pH}(t+1)^1 \ldots \mathrm{pH}(t+1)^n - \mathrm{pH}(t)^1 \ldots - \mathrm{pH}(t)^n - C_{rc}(t-1)]$$

The unknown parameters can be estimated using the following recursive parameter adaptation algorithm:

$$\hat{\boldsymbol{\theta}}_j(t+1) = \hat{\boldsymbol{\theta}}_j(t) + F(t)\,\boldsymbol{\phi}(t) \times [1 + \boldsymbol{\phi}^T(t)\, F(t)\, \boldsymbol{\phi}(t)]^{-1} \times \eta^0(t+1)$$

$$F^{-1}(t) = \lambda_1(t)\, F^{-1}(t-1) + \lambda_2(t)\, \boldsymbol{\phi}(t)\, \boldsymbol{\phi}^T(t)$$

$$\eta^0(t) = C_{rc}(t-1) - \sum_{j=1}^{m} \psi_j \hat{\boldsymbol{\theta}}_j^T(t-1) \times \boldsymbol{\phi}(t-1) = C_{rc}(t-1) - \hat{C}_{rc}^0(t) \quad (13)$$

with

$$F(0) > 0;\quad 0 < \lambda_1(t) \leq 1;$$
$$0 \leq \lambda_2(t) < 2$$

Simulation and experimental results of identification of a pH-process represented by model (6) and using algorithm (13) are given in [13]. Substituting the unknown parame-

ters with their estimates in Eq. (11), the adaptive control law yields

$$C_{rc}(t) = \sum_{j=1}^{m} \psi_j [\hat{\theta}_j^T(t)\, \phi_1(t)] \qquad (14)$$

A schematic block diagram of this adaptive control scheme is presented in Fig. 3. Note that, in some cases, automatic adjustment of the model reference was needed to improve the operation of the proposed adaptive control scheme shown in Fig. 3, as shown in the simulation test results discussed later.

Second Scheme

The second scheme is based on the model in Fig. 4. The linear dynamic part of the model is given by Eq. (4). The main reason for the changes in the parameters a_1, b_0, and b_1 is the change of the flow F. Measuring the flow F allows determination of new values of the parameters. The linear controller is designed based on pole-placement principles [8].

The nonlinear inverse approximation is given by Eq. (5), and the parameters γ_{ji} are estimated in closed loop, using a least-squares algorithm.

Simulation Results

First Scheme

Tracking of a Sinusoidal Reference Signal The process block is the simulated pH-process with the concentrations of the components corresponding to the process feed III (Fig. 2) for the first 150 min and to process feed I from 150 to 300 min. The best results, shown in Fig. 5, are obtained when the nonlinearity is approximated by a piecewise-cubic function with three intervals with breakpoints at $pH_1 = 5.4$, $pH_2 = 6.4$, and $pH_3 = 8$.

The time constant of the reference model is 0.3 min. The initial adaptation gain is diagonal (10), and it is always reinitialized when the process feed changes.

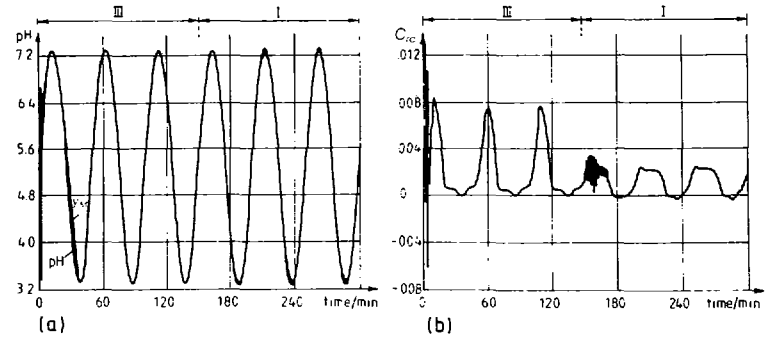


Fig. 5. Tracking of a sinusoidal reference signal. (a) Process and reference model outputs. (b) Reagent concentration.

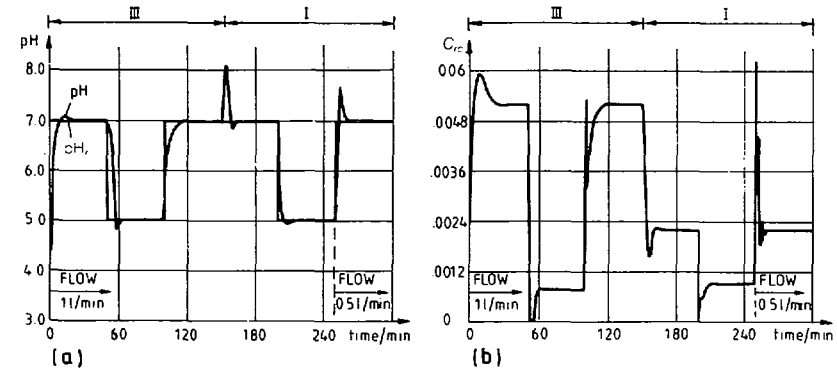


Fig. 6. Tracking of a piecewise-constant reference using the control scheme shown in Fig. 3. (a) Process and reference model outputs. (b) Reagent concentration.

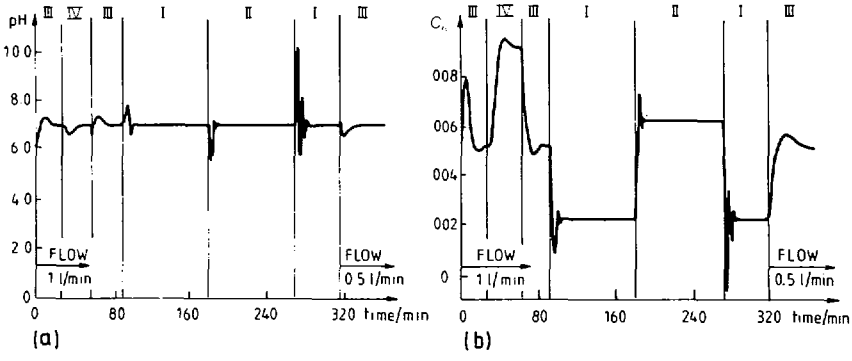


Fig. 7. Regulation results using the control scheme shown in Fig. 3 for process feeds I–IV. (a) Process output. (b) Reagent concentration.

Tracking of a Piecewise-Constant Reference Signal The same adaptive scheme, but provided with an integral mode [14], is used. The best results, shown in Fig. 6, are obtained when the nonlinearity is approximated by a piecewise-linear function with two intervals with breakpoints at $pH_1 = 6.2$ and $pH_2 = 8$. The time constant of the reference model is 1.6 min, and the sampling time is 0.5 min. The process steady-state gain for feed I changes 5-fold, and for feed II changes 11-fold for the considered set points.

Regulation The same scheme with the integral mode is used with the concentration disturbances shown in Fig. 7. The steady-state gains of the process feeds at pH equal 7 are: 4235, 5333, 180, and 200, respectively, for the four different process feeds I, II, III, and IV (see Table). The best results are obtained using a linear approximation of the nonlinearity; the time constant of the reference model is 1.6 min, and the sampling time is 0.5 min.

Next, a more difficult process is simulated, such that the titration curves are steeper and the nonlinearities are more severe. Influent changes from acidic to basic and reverse are also treated. The steady-state gains of the process feeds at pH equal 7 are 24,039 for the feeds V and VI, 475 for the feeds VII and VIII, and 3712 for the feed IX. The concentration disturbances corresponding to different process feeds are marked in Figs. 8–10. The classical proportional-integral (PI) controller fails in this case, as shown in Fig. 8. The best simulation results, shown in Fig. 9, are obtained using a linear adaptive controller. The initial gain is diagonal (1). The parameter estimates and the matrix gain are initialized when the influent pH is changed.

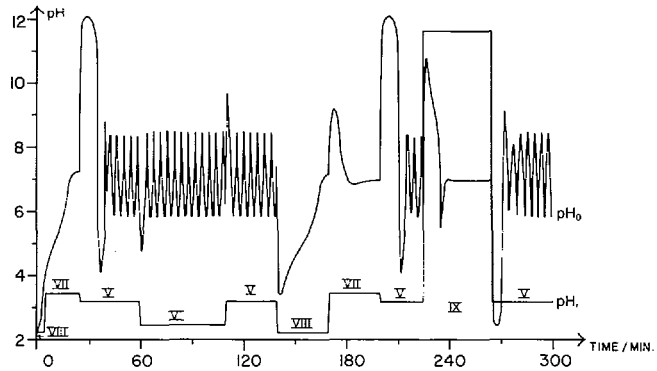


Fig. 8. Regulation results using the PI controller with fixed parameters (K_p = 0.0015, T_I = 1.0) for process feeds V–IX.

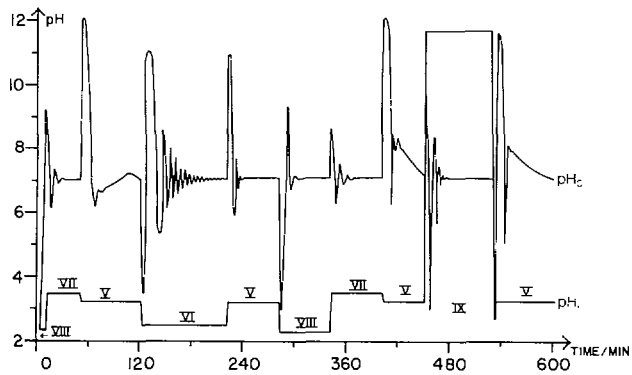


Fig. 9. Regulation results using the adaptive scheme shown in Fig. 3 for process feeds V–IX.

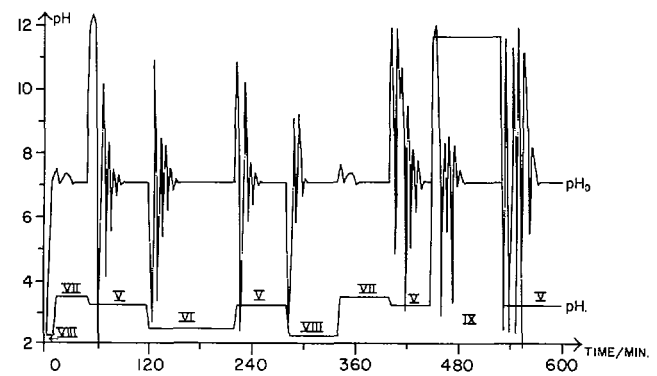


Fig. 10. Regulation results using the control scheme shown in Fig. 4 for process feeds V–IX.

The sampling time is 0.5 min. The time constant of the reference model is always set to 2 min after every change of influent pH. It is automatically increased by two if large oscillations are detected without the change of the influent from acidic to basic or reverse. If the change of influent from basic to acidic or from acidic to basic is detected, then the reagent flow is immediately changed from strong base to strong acid or from strong acid to strong base, respectively.

Second Scheme

Finally, it was assumed that the parameters of the dynamic part of the model are initially known and can be adapted in the feedforward loop based on the flow measurements. Hence, only the coefficients of the piecewise-polynomial approximation of the static nonlinearity are adapted in the closed loop. In this case, the linear controller works only if the zeroth-order coefficient in the polynomial approximation of the nonlinearity, which is in fact known a priori, is also estimated. The initial matrix gain is diagonal (10,000).

The best results for step responses are obtained when a controller is designed using model following control method, with model reference time constant 2 min, sampling time 0.5 min, and a linear approximation of the static nonlinearity. When the controller was designed using the pole-placement method with the desired closed-loop polynomial $A^*(q^{-1}) = (1-0.1q^{-1})^3$, the best step responses for feeds V–VIII were obtained for the sampling time of 1.5 min and the linear approximation of the titration curve. However, for feed IX, the best result is obtained using the nonlinear approximation of the titration curve and the sampling time of 1.25 min. When the linear approximation is used, slightly worse response is obtained for the sampling time of 1.5 min. However, for the sampling time of 1.25 min, this linear controller does not work at all for feed IX. On the other hand, this scheme with the nonlinear approximation works quite well for all feeds, except VI. For feed VI, it converges only if additional perturbations are added at the process input.

The best results for the series of step changes in the process feed are obtained using the linear controller designed based on the pole-placement method, the linear approximation of the titration curves, and the sampling time of 1.5 min, as shown in Fig. 10. The estimates and the gain matrix are initialized always when the pH of influent has changed.

The computer control system, implemented at the Control Engineering Laboratory of Helsinki University of Technology, was used for experimental checking of the theoretical and simulation results presented above. Most of the experimental test results corresponded to the simulation results, as reported in [14], [15].

Conclusions

Different adaptive control schemes are used for tracking and regulating difficult pH-processes. The process considered is so difficult that the classical PID controller does not work at all. The model reference adaptive control scheme with a time-varying reference model has to be used in order to obtain correct results. In the case when the linear dynamics of the process is considered

known and only the titration curve is identified, the regulation results are more oscillatory than when the parameters of the linear dynamic model are estimated simultaneously with the coefficients of the piecewise-polynomial approximation of the titration curve. This means that when the first scheme shown in Fig. 3 is used, more parameters have to be estimated, but better performance is obtained than using the second scheme shown in Fig. 4. For that reason, it is recommended that the first scheme be used for control of any Wiener-type nonlinear systems with time-varying parameters.

Comparing the performance of a linear and a nonlinear adaptive controller, it was shown that when the titration curve is very nonlinear in the operation range, then the nonlinear adaptive controller works better than the linear one for tracking as well as for regulation purposes when infrequent disturbances in process feed occur. Even if the breakpoints are not chosen in an optimal way, it is still better to use the nonlinear controller rather than the linear one in these cases. However, when the titration curve changes very often and varies widely, as in the case of frequent step disturbances, the nonlinear adaptive controller does not work correctly and the linear adaptive controller should be used.

Acknowledgments

The author gratefully acknowledges the help of Dr. Pentti Jutila from the Helsinki University of Technology for choosing suitable pH-process solutions, and Pekka Jakkola for performing the simulation tests.

References

[1] V. L. Trevathan, "Advanced Control of pH," ISA Annual Conf., Paper No. 839, Philadelphia, PA, pp. 62-68, 1978.

[2] V. L. Trevathan, "Characteristics of a pH Control," *Proc. of the Workshop on Industrial Process Control*, Tampa, FL, AIChE, NY, pp. 24-28, 1979.

[3] F. G. Shinskey, *pH and pION Control in Process and Waste Streams*, New York: Wiley, 1973.

[4] F. Bucholt and M. Kummel, "Self-Tuning Control of a pH-Neutralization Process," *Automatica*, vol. 15, pp. 665-671, 1979.

[5] S. Bermann and K. H. Lachmann, "Digital Parameter Adaptive Control of a pH Process," Joint Autom. Control Conf., San Francisco, CA, 1980.

[6] F. G. Shinskey, "A Self-Adjusting System for Effluent pH Control," Spring Joint Conf. ISA, St. Louis, MO, 1978.

[7] C. G. Proudfoot, D. W. Clarke, O. L. R. Yardos, and P. S. Tuffs, "Comparative Study of Self-Tuning Controllers Regulating pH in an Industrial Process," *Proc. of IEE Conf. Control 85*, Cambridge, 1985.

[8] G. C. Goodwin and K. S. Sin, *Adaptive Filtering, Prediction and Control*, Englewood Cliffs, NJ: Prentice-Hall, 1984.

[9] P. Jutila and A. Visala, "Pilot Plant Testing of an Adaptive pH-Control Algorithm Based on Physico-Chemical Modelling," *Mathematics and Computers in Simulation*, vol. XXVI, pp. 523-533, 1984.

[10] A. Niemi and P. Jutila, "pH Control by Linear Algorithms," *5th IFAC/IFIP Conf.*, The Hague, Proc., North Holland, 1977.

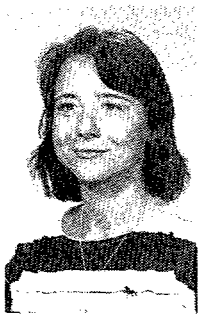
[11] P. K. Jutila, G. A. Pajunen, and A. J. Niemi, "Computer Control of pH Reactor," 1985 Amer. Control Conf., pp. 1165-1370, June 19-21, 1985.

[12] I. D. Landau, "Deterministic and Stochastic Adaptive Pole-Zero Placement for Minimum Phase Systems," *Richerche di Automatica*, vol. 8, no. 1, pp. 140-171, 1982.

[13] G. A. Pajunen, "Recursive Identification of Wiener Type Nonlinear Systems," 1985 Amer. Control Conf., pp. 1365-1370, June 19-21, 1985.

[14] G. A. Pajunen, "Application of a Model Reference Adaptive Technique to the Identification and Control of Wiener Type Nonlinear Processes," *Acta Polytechnica Scandinavica*, Electrical Engineering Series No. 52, Helsinki, 1984.

[15] P. Jaakola, "Adaptive pH-Controllers," master's thesis, Helsinki University of Technology, Department of Electrical Engineering, 1986 (in Finnish).



Grazyna A. Pajunen was born in Warsaw, Poland. She received the M.Sc. degree in electronics from the Warsaw Technical University, Warsaw, Poland, in 1975, the Licenciate degree of technology and the Ph.D. degree from the Helsinki University of Technology, Helsinki, Finland, in 1980 and 1984, respectively. From 1975 to 1979, she was a Design Engineer for the electrical firm of Oy Stromberg Ab in Helsinki, Finland. From 1979 to 1985, she was a teaching and research assistant at Helsinki University of Technology, investigating problems concerned with identification and adaptive control of Wiener-type nonlinear systems, in general, and of the pH-process in continuous-flow reactors, in particular. At present, she is an Assistant Professor in the Electrical and Computer Engineering Department at Florida Atlantic University, Boca Raton, Florida. Her current interests include control systems, system identification, adaptive control, and robotics.