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ADAPTIVE INPUT–OUTPUT LINEARIZATION OF A pH NEUTRALIZATION PROCESS

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SUMMARY

Adaptive non-linear control strategies for a pH neutralization process are developed and evaluated via simulation. A non-adaptive non-linear controller is designed using a modified input–output linearization technique which accounts for the implicit output equation in the reaction invariant model. For simplicity the reaction invariants are assumed to be available for feedback. Because the model exhibits significant time-varying behaviour, the input–output linearizing controller is combined with non-linear parameter estimators which account for unmeasured buffering changes. Simulation results demonstrate that a novel indirect adaptive strategy is most suitable for experimental implementation where the reaction invariants must be estimated and sampling is required. © 1997 by John Wiley & Sons, Ltd.

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1. INTRODUCTION

pH control is critical in a variety of chemical and biological process but is notoriously difficult.[1,2] These control problems are attributable to both non-linear and time-varying process characteristics. Industrial pH neutralization systems often exhibit severe static non-linearities, because the titration curve varies by several orders of magnitude over a modest range of pH values. Moreover, the titration curve may be time-varying owing to changes in buffering. As discussed in Section 2, a variety of control strategies have been proposed for pH neutralization processes. However, most of these techniques neglect important non-linear and/or time-varying characteristics. As a result, pH control strategies which are both non-linear and adaptive are needed.

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In this paper, adaptive non-linear control strategies are developed for a pH neutralization process. The controller design is based on a reaction invariant model of the UCSB pH neutralization system. In this study the reaction invariants are assumed to be available for feedback. Three adaptive non-linear controllers are developed by combining an input–output linearizing controller with non-linear parameter estimators which predict the buffering content of the system. The three adaptive controllers are compared via simulation for setpoint changes and unmeasured disturbances.

The paper is organized as follows. In Section 2 a survey of existing pH control strategies is presented. The reaction invariant model and simulation results for a PI controller are presented in Section 3. In Section 4 the design of the adaptive non-linear controllers is described and comparative simulation results are presented. Conclusions are presented in Section 5.

2. SURVEY OF pH CONTROL STRATEGIES

pH control techniques can be conveniently classified as non-adaptive linear, adaptive linear, non-adaptive non-linear and adaptive non-linear. Non-adaptive linear control strategies such as PID control can be expected to provide adequate performance if the process is operated near the region where the controller was tuned and buffering variations are small.[3] Otherwise the controller must be tuned conservatively to ensure stability for high-gain conditions and sluggish performance is obtained for other operating regimes.[4,5] Sliding mode control strategies provide a possible solution to this dilemma but often suffer from manipulated input chattering.[6] If the titration curve is known a *priori*, a linear gain-scheduled controller can provide satisfactory performance.[1] However, the titration curve usually varies owing to unmeasured changes in buffering.

A variety of linear adaptive control strategies have been proposed to account for time-varying process characteristics. Several techniques are based on self-tuning control of empirical discrete-time models.[7,8] In practice it may be advantageous to adapt only the steady state gain instead of the entire dynamic model, since most pH systems exhibit nearly linear dynamics but severe static non-linearities.[4,9,10] Adaptive linear control schemes based on gain scheduling[11–13] and predictive control[14,15] have also been proposed. The major shortcoming of these approaches is the use of a linear process model. It is difficult to handle severe process non-linearities by reparametrizing a linear model for different operating points.

Non-linear process characteristics can be addressed explicitly using non-linear control strategies. Most of these techniques are based on non-linear state space models and therefore require state feedback. State estimation is not required for strong acid, strong base neutralizations, because the model contains a single state variable which is easily determined from the pH. Several non-adaptive non-linear control strategies based on input–output linearization have been proposed for strong acid, strong base systems.[16–18] However, these techniques are not applicable to buffered systems, which typically require state estimation.

Adaptive non-linear control strategies which are applicable to buffered processes have been developed by Gustafsson and Waller.[19,20] Indirect pH control is achieved by regulating a 'reaction invariant' which is estimated with a recursive least squares scheme. This approach has been shown to provide superior regulatory performance to conventional PID and linear adaptive control.[21,22] A similar technique has been proposed by Jutilia.[23] However, this approach is based on the unrealistic assumption that the estimated reaction invariant is slowly varying. Moreover, a pH measurement of the feed stream is often required for successful implementation.[21]

A closely related non-adaptive control strategy has been developed by Wright and Kravaris.[24] Their technique is based on reformulating the pH control problem in terms of a weighted sum of ionic concentrations termed the 'strong acid equivalent'. This transformed output provides a nearly linear control problem. Experimental results for bench-scale and industrial processes have been presented.[25,26] However, even under ideal conditions (e.g. no buffering changes) this approach does not ensure good transient performance, because the strong acid equivalent is a non-linear function of the pH. Moreover, the technique is non-adaptive and therefore does not address buffering changes.

Parrish and Brosilow[27] have applied an adaptive non-linear control strategy based on input–output linearization to a buffered pH model. The proposed technique yields superior control to a PID controller. Li and Biegler[28] achieve similar performance improvements for the same model using an adaptive Newton-type controller. However, in both these techniques the control actions are generated using iterative calculations, which may not converge. An alternative adaptive control strategy based on input–output linearization has been developed by Williams *et al.*[29] This technique can yield poor transient performance, because parameter estimation is performed only when the system is operating near steady state conditions. This brief survey demonstrates that the non-linear and time-varying characteristics of pH neutralization processes are not adequately addressed by existing control strategies.

3. THE PROCESS MODEL AND PI CONTROL

3.1. The Process model

A simplified schematic diagram of the UCSB bench-scale pH neutralization system is shown in Figure 1. The process consists of an acid steam (q_1), buffer stream (q_2) and base stream (q_3) which are mixed in a tank. The objective is to regulate the effluent pH (pH_4) by manipulating the base flow rate; the acid and buffer flow rates are considered as unmeasured disturbances. The dynamic model of the pH neutralization process is derived using conservation equations and equilibrium relations.[4,5] Modelling assumptions include negligible actuator and transmitter dynamics, constant fluid volume (V), perfect mixing, constant density and complete solubility of the ions involved. The chemical reactions are

$$H_2CO_3 \leftrightarrow HCO_3^- + H^+ \tag{1}$$

$$HCO_3^- \leftrightarrow CO_3^{2-} + H^+ \tag{2}$$

$$H_2O \leftrightarrow OH^- + H^+ \tag{3}$$

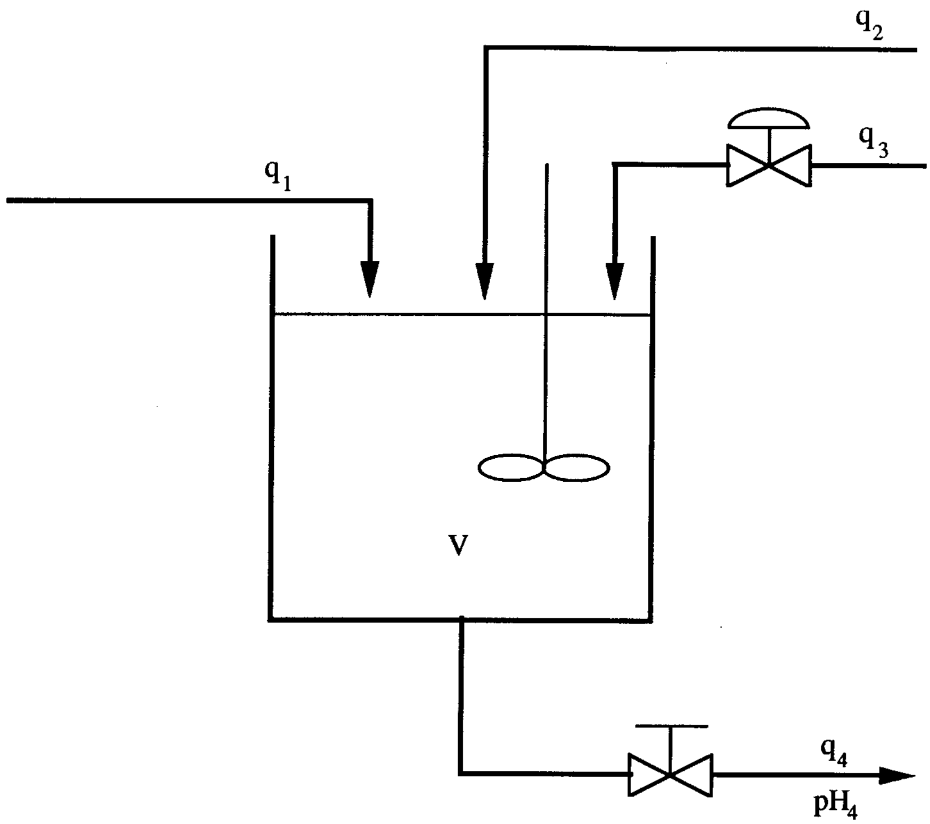

Figure 1. The UCSB pH neutralization process

The equilibrium constants for the reactions are

$$K_{a1} = \frac{[HCO_3^-][H^+]}{[H_2CO_3]} \tag{4}$$

$$K_{a2} = \frac{[CO_3^{2-}][H^+]}{[HCO_3^-]} \tag{5}$$

$$K_w = [H^+][OH^-] \tag{6}$$

The chemical equilibria are modelled using the reaction invariant approach.[19,30] For the UCSB system, two invariants are defined for each inlet stream ($i = 1, 2, 3$):

$$W_{ai} = [H^+]_i - [OH^-]_i - [HCO_3^-]_i - 2[CO_3^{2-}]_i \tag{7}$$

$$W_{bi} = [H_2CO_3]_i + [HCO_3^-]_i + [CO_3^{2-}]_i \tag{8}$$

The invariant W_a is a charge-related quantity, while W_b represents the concentration of the carbonate ion. Unlike the pH, these invariants are independent of the extent of the reactions in (1)–(3) and therefore are conserved quantities. The hydrogen ion concentration can be determined from W_a and W_b:[4]

$$W_b \frac{K_{a1}/[H^+] + 2K_{a1}K_{a2}/[H^+]^2}{1 + K_{a1}/[H^+] + K_{a1}K_{a2}/[H^+]^2} + W_a + \frac{K_w}{[H^+]} - [H^+] = 0 \tag{9}$$

The pH is related to the hydrogen ion concentration as

$$pH = -\log([H^+]) \tag{10}$$

If the reaction invariants of a stream are known, the pH of the stream can be determined by solving the non-linear equations (9) and (10). By combining mass balances on each of the ionic species in the system, the following differential equations for the effluent reaction invariants (W_{a4}, W_{b4}) can be derived:[4]

$$V\frac{dW_{a4}}{dt} = q_1(W_{a1} - W_{a4}) + q_2(W_{a2} - W_{a4}) + q_3(W_{a3} - W_{a4}) \tag{11}$$

$$V\frac{dW_{b4}}{dt} = q_1(W_{b1} - W_{b4}) + q_2(W_{b2} - W_{b4}) + q_3(W_{b3} - W_{b4}) \tag{12}$$

Table I. Nominal operating conditions for pH process

$V = 2900$ ml	$q_3 = 15{\cdot}6$ ml s^{-1}
$K_{a1} = 4{\cdot}47 \times 10^{-7}$	$W_{a1} = 0{\cdot}003$ M
$K_{a2} = 5{\cdot}62 \times 10^{-11}$	$W_{b1} = 0$ M
$K_w = 1 \times 10^{-14}$	$W_{a2} = -0{\cdot}03$ M
$\Delta t = 1$ s	$W_{b2} = 0{\cdot}03$ M
$[q_1] = 0{\cdot}003$ M HNO_3	$W_{a3} = -3{\cdot}05 \times 10^{-3}$ M
$[q_2] = 0{\cdot}03$ M $NaHCO_3$	$W_{b3} = 5{\cdot}00 \times 10^{-5}$ M
$[q_3] = 0{\cdot}003$ M NaOH,	$W_{a4} = -4{\cdot}32 \times 10^{-4}$ M
5×10^{-5} M $NaHCO_3$	$W_{b4} = 5{\cdot}28 \times 10^{-4}$ M
$q_1 = 16{\cdot}6$ ml s^{-1}	$pH_4 = 7.00$
$q_2 = 0{\cdot}55$ ml s^{-1}	

Table II. Lists of figures for closed-loop simulations tests

Controller	Setpoint changes	Buffer changes	Acid changes	Buffer changes ($\Delta t = 15$ s)
PI	5	6	—	7
Non-adaptive	8	10	9	—
Direct adaptive	11, 12	13	—	14[a]
Indirect adaptive #1	—	15	—	16
Indirect adaptive #2	—	17	18	19

[a] $\Delta t = 5$ s.

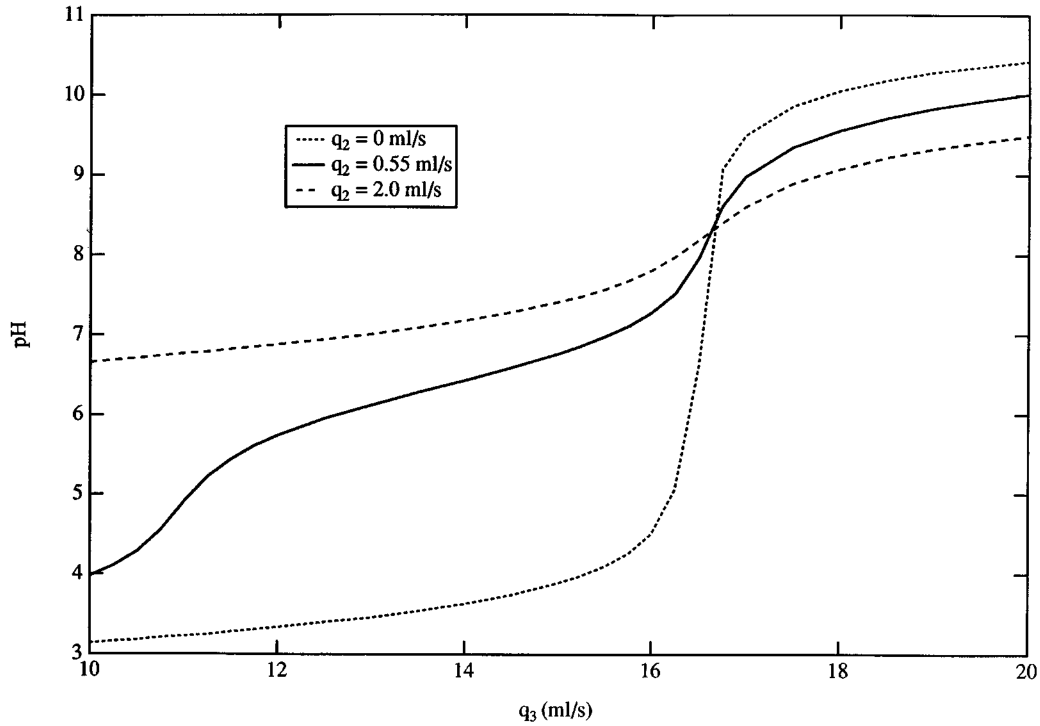

Figure 2. Titration curves for three buffer flow rates

The nominal sampling period is $\Delta t = 1$ s. A complete set of the nominal model parameters and operating conditions is given in Table I, while a list of figures for the closed-loop tests is provided in Table II.

3.2. Open-loop behaviour

Titration curves for three buffer flow rates are shown in Figure 2. Note that the process gain at a particular operating point is the slope of the titration curve at that point. For the nominal buffer flow rate ($q_2 = 0{\cdot}55$ ml s^{-1}) the process gain varies by almost 1000% over the region shown. Moreover, the titration curves for $q_2 = 0$ and $2{\cdot}0$ ml s^{-1} are dramatically different from the curve obtained under nominal conditions.

The open-loop pH response for base flow rate changes and nominal buffering conditions is shown in Figure 3. The sequence of flow rate changes is shown in the top half of the figure. Although the step changes are symmetrical ($\pm 2{\cdot}0$ ml s^{-1}), the pH responses are highly asymmetric owing to static non-linearities. Similar results are obtained for acid flow rate changes.[31] The open-loop pH response for a series of buffer flow rate changes is shown in Figure 4. Note that large changes in q_2 can yield relatively small pH variations. By contrast, when the buffer flow rate is set to $q_2 = 0$ ml s^{-1}, a very large change in the pH results, because the system has almost no buffering capacity. These simulation results demonstrate that the pH neutralization model is very non-linear and exhibits significant time-varying behaviour if the buffer flow rate varies.

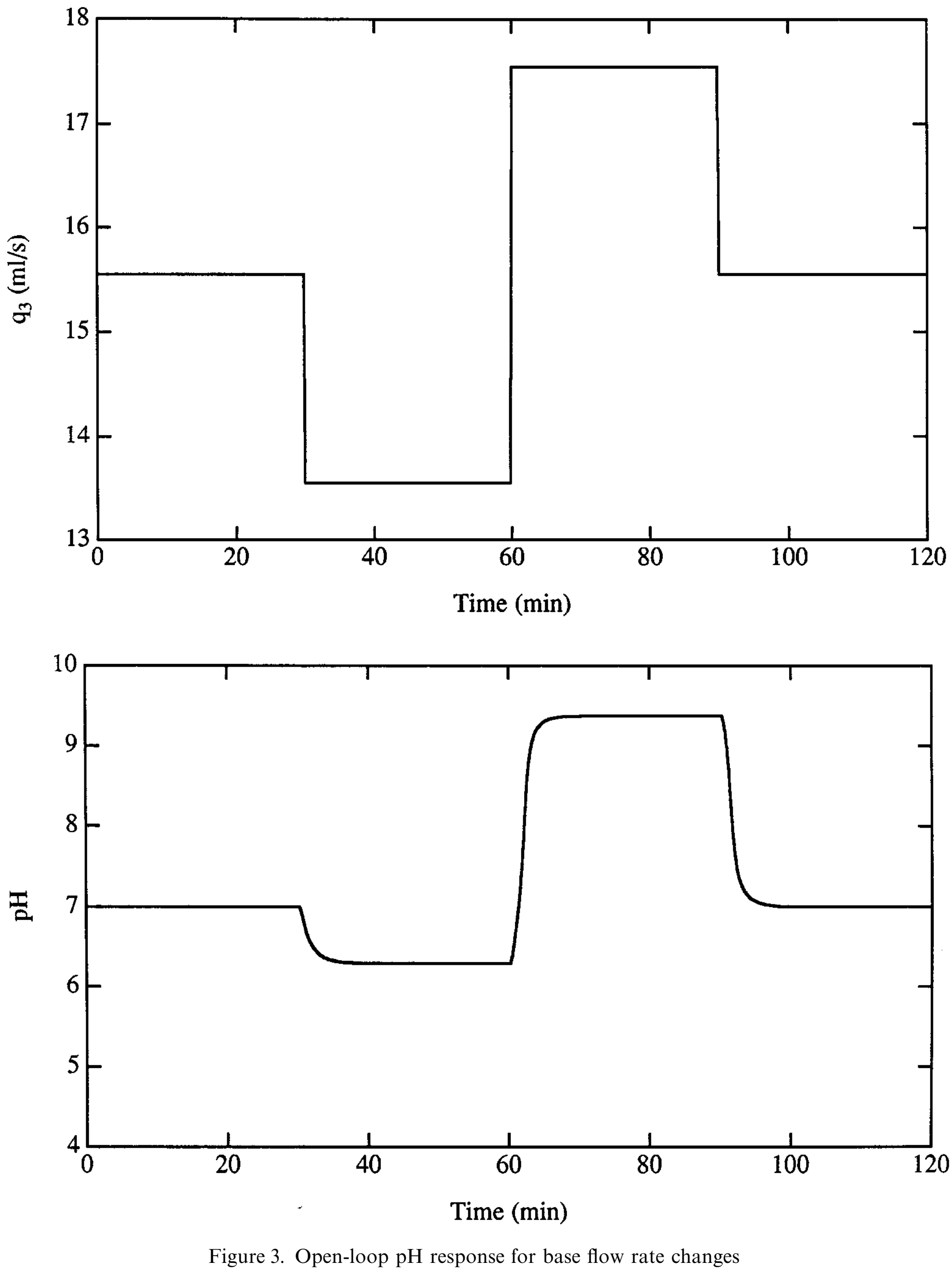

Figure 3. Open-loop pH response for base flow rate changes

3.3. PI control

Although PI control does not explicitly account for non-linear or time-varying process characteristics, it is often used in practice and provides a valuable benchmark to evaluate the

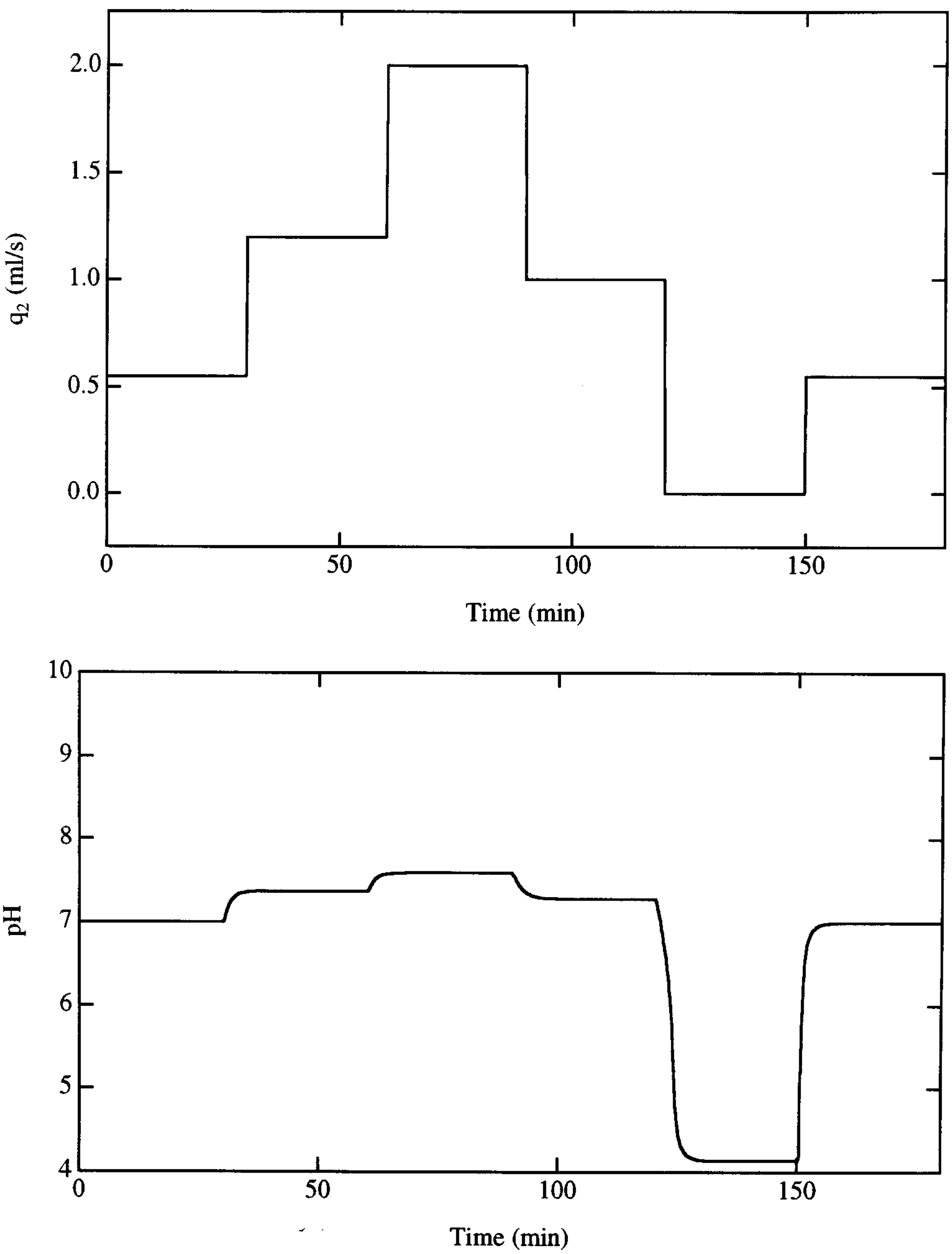

Figure 4. Open-loop pH response for buffer flow rate changes

adaptive non-linear controllers presented in Section 4. The PI controller parameters were initially determined using internal model control (IMC) tuning rules[32] for two first-order models obtained from the open-loop responses in Figure 3. The IMC closed-loop time constant was chosen to be 0·75 min, which is roughly one-half the open-loop time constants. The final

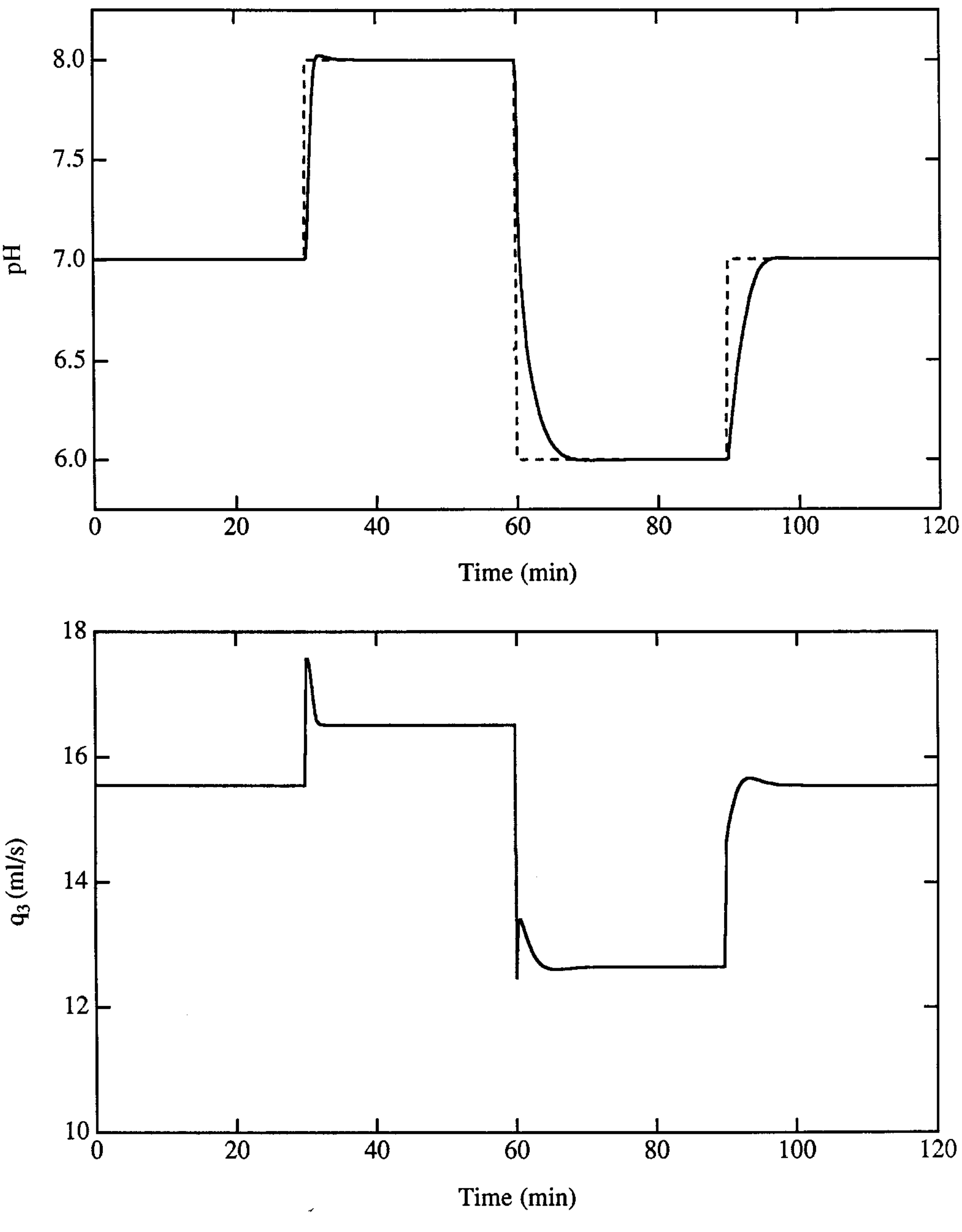

Figure 5. PI control for setpoint changes

controller parameters $K_c = 2{\cdot}0$ ml s^{-1} and $\tau_I = 100$ s were chosen to provide reasonable setpoint responses.

The setpoint tracking performance of the PI controller is shown in Figure 5 along with the pH setpoint (broken line). The controller tracks the first setpoint change quickly, while relatively sluggish responses are obtained for subsequent changes. The performance of the PI controller for

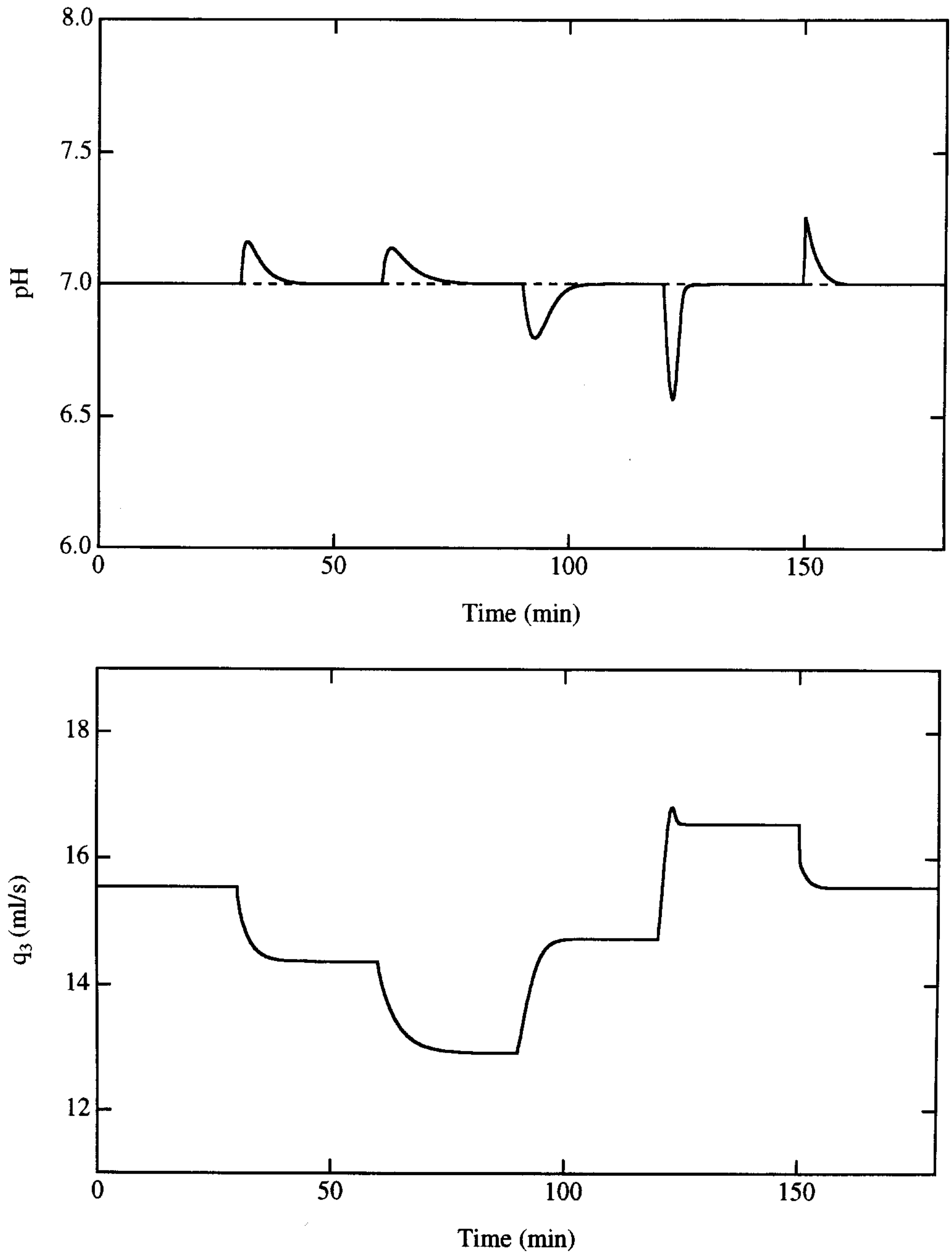

Figure 6. PI control for buffer flow rate disturbances

the q_2-disturbances in Figure 4 is shown in Figure 6. The responses are generally sluggish; however, a rapid response is obtained when $q_2 \to 0$ ml s^{-1}, which represents a high-gain condition (see Figure 2). The performance of the PI controller for the same sequence of q_2-disturbances when the sampling period is increased to $\Delta t = 15$ s is shown in Figure 7.

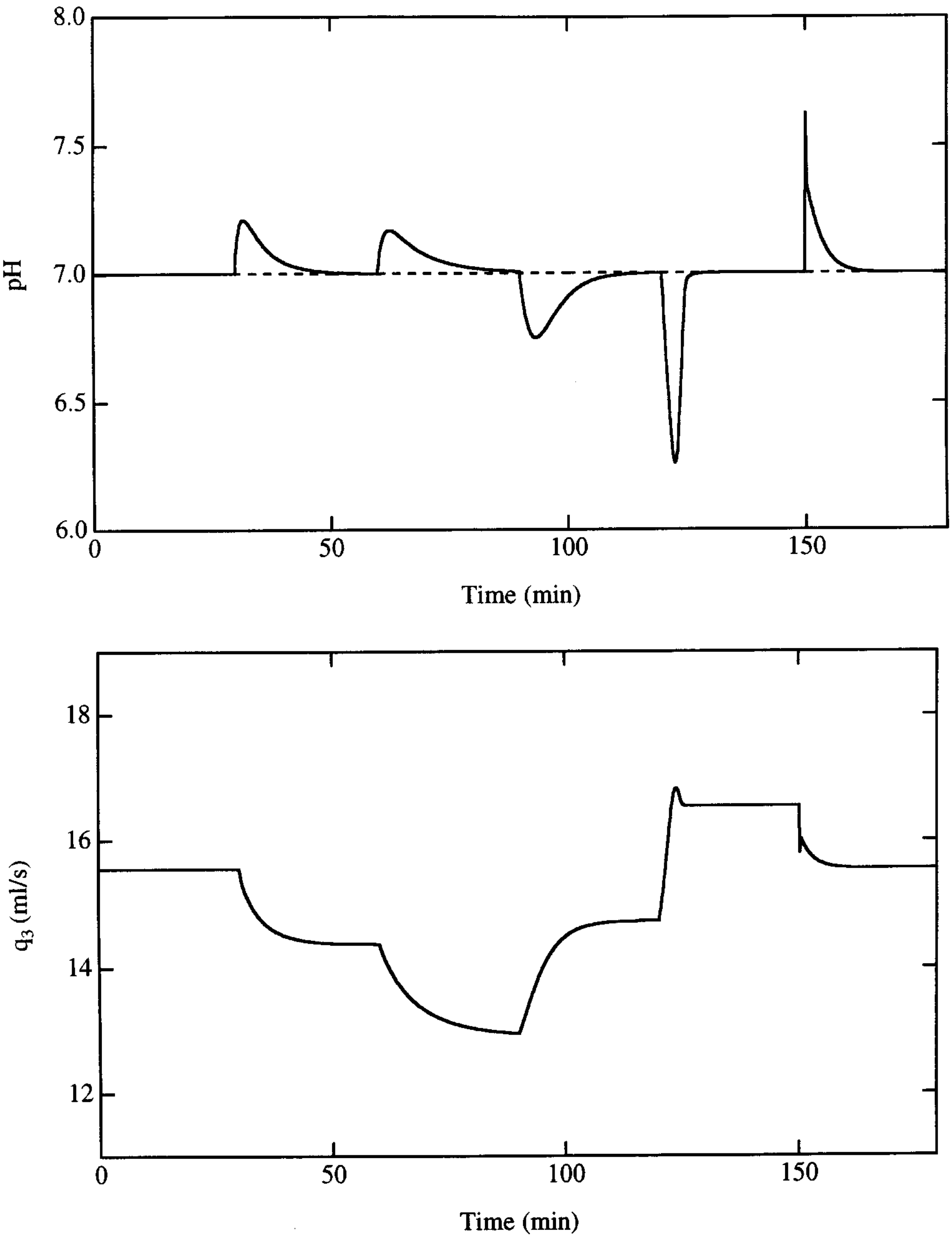

Figure 7. PI control with $\Delta t = 15$ s for buffer flow rate disturbances

This sampling period is the nominal value used experimentally.[31] The PI controller gain must be reduced to $K_c = 1{\cdot}0$ ml s^{-1} in order to maintain stability when $q_2 \rightarrow 0$ ml s^{-1}. As a result, the pH responses are even more sluggish than in the case where $\Delta t = 1$ s. Hence a well-tuned PI controller does not provide satisfactory performance for this pH neutralization process.

4. ADAPTIVE NON-LINEAR CONTROL

4.1. Non-adaptive non-linear control

A non-linear state space representation of the pH neutralization model can be obtained by defining the state variables, disturbance, input and output as

$$x \triangleq [W_{a4} \quad W_{b4}]^{T}, \qquad d \triangleq q_2, \qquad u \triangleq q_3, \qquad y \triangleq \mathrm{pH} \tag{13}$$

In this case the process model (9)–(12) has the form

$$\dot{x} = f(x) + g(x)u + p(x)d \tag{14}$$

$$c(x, y) = 0 \tag{15}$$

where

$$f(x) = \left[\frac{q_1}{V}(W_{a1} - x_1) \quad \frac{q_1}{V}(W_{b1} - x_2) \right]^{T} \tag{16}$$

$$g(x) = [\frac{1}{V}(W_{a3} - x_1) \quad \frac{1}{V}(W_{b3} - x_2)]^{T} \tag{17}$$

$$p(x) = [\frac{1}{V}(W_{a2} - x_1) \quad \frac{1}{V}(W_{b2} - x_2)]^{T} \tag{18}$$

$$c(x, y) = x_1 + 10^{y-14} - 10^{-y} + x_2 \frac{1 + 2 \times 10^{y - \mathrm{p}K_2}}{1 + 10^{\mathrm{p}K_1 - y} + 10^{y - \mathrm{p}K_2}} \tag{19}$$

In (19), $\mathrm{p}K_1 = \log(K_{a1})$ and $\mathrm{p}K_2 = \log(K_{a2})$.

Note that the output equation (19) is an implicit function of the output y. As a result, standard input–output linearization techniques[33,34] are not directly applicable to the pH neutralization model. However, an input–output linearizing controller can be designed for (14)–(19) as follows.[16,35] Taking the derivative of the output equation along the system trajectories and rearranging the resulting equation yields

$$\dot{y} = -c_y^{-1}(x, y)c_x(y)[f(x) + g(x)u + p(x)d] \tag{20}$$

where the partial derivatives are

$$c_x(y) = [1 \quad \frac{1 + 2 \times 10^{y - \mathrm{p}K_2}}{1 + 10^{\mathrm{p}K_1 - y} + 10^{y - \mathrm{p}K_2}}]^{T} \tag{21}$$

$$c_y(x, y) = (\ln 10)\left(10^{y-14} + 10^{-y} + x_2 \frac{10^{\mathrm{p}K_1 - y} + 10^{y - \mathrm{p}K_2} + 4(10^{\mathrm{p}K_1 - y})(10^{y - \mathrm{p}K_2})}{(1 + 10^{\mathrm{p}K_1 - y} + 10^{y - \mathrm{p}K_2})^2}\right) \tag{22}$$

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 standard input–output linearization techniques can be applied to (20). The approach is easily extended to models with relative degree $r \geqslant 1$.

Assuming the reaction invariants are available for feedback, the input–output linearizing controller is obtained by solving the following equation for u:

$$-c_y^{-1}(x,y)c_x(y)[f(x)+g(x)u+p(x)\hat{d}]=v \tag{23}$$

where $\hat{d}$ is the estimated value of the buffer flow rate and the new input v is chosen as[34]

$$v=-2\varepsilon^{-1}y+\varepsilon^{-2}\int_0^t (y_{\mathrm{sp}}-y)\,\mathrm{d}\tau \tag{24}$$

In (24), y_{sp} is the pH setpoint and ε is the controller tuning parameter. Because (23) is affine in u, the input–output linearizing controller can be written as

$$u=\frac{\varepsilon^{-2}\int_0^t (y_{\mathrm{sp}}-y)\mathrm{d}\tau-2\varepsilon^{-1}y+c_y^{-1}(x,y)c_x(y)\,[f(x)+p(x)\hat{d}]}{-c_y^{-1}(x,y)c_x(y)g(x)} \tag{25}$$

The non-adaptive version of the controller uses the nominal value of the buffer flow rate, $\hat{d}=0{\cdot}55$ ml s^{-1}.

In the absence of modelling errors the non-linear control low in (25) yields the closed-loop transfer function (CLTF)

$$\frac{y(s)}{y_{\mathrm{sp}}(s)}=\frac{1}{(\varepsilon s+1)^2} \tag{26}$$

The output is asymptotically stable as long as $0\leqslant\varepsilon<\infty$. The nominal value $\varepsilon=0{\cdot}75$ min used in this study is approximately one-half the open-loop time constant for the open-loop responses in Figure 3. The input and state variables are also asymptotically stable if the zero dynamics are bounded-input, bounded-state stable.[33,34] In practice this condition is difficult to check; however, extensive simulation studies indicate that the zero dynamics of the pH neutralization model are asymptotically stable in all operating regions of practical interest.[31]

The setpoint tracking performance of the non-adaptive non-linear controller when the buffer flow rate is known exactly is shown in Figure 8. Note that the pH response follows the CLTF in (26) and the non-linear controller outperforms the PI controller (Figure 5) for the last two setpoint changes. The regulatory performance of the non-linear controller for a series of unmeasured acid flow rate disturbances is shown in Figure 9. The disturbance sequence is identical with that in Figure 3 for the base flow rate except that $\pm 2{\cdot}0$ ml s^{-1} changes from the nominal acid flow rate $q_1=16{\cdot}6$ ml s^{-1} are employed. The non-linear controller provides improved disturbance rejection as compared with the PI controller (not shown) while using reasonable control moves.

The performance of the non-adaptive non-linear controller can deteriorate markedly for buffer flow rate variations. This behaviour is shown in Figure 10 for the unmeasured buffer flow rate disturbances in Figure 4. The pH response of the non-linear controller is superior to that of the PI controller (Figure 6) for all conditions except when $q_2\rightarrow 0$ ml s^{-1}. In this case a highly oscillatory response is obtained, because the controller generates overly aggressive control moves as a result of the large increase in the process gain. Although acceptable control is obtained if $q_2\geqslant 0{\cdot}1$ ml s^{-1}, this result demonstrates that the non-adaptive non-linear controller is unacceptable for large buffering changes.

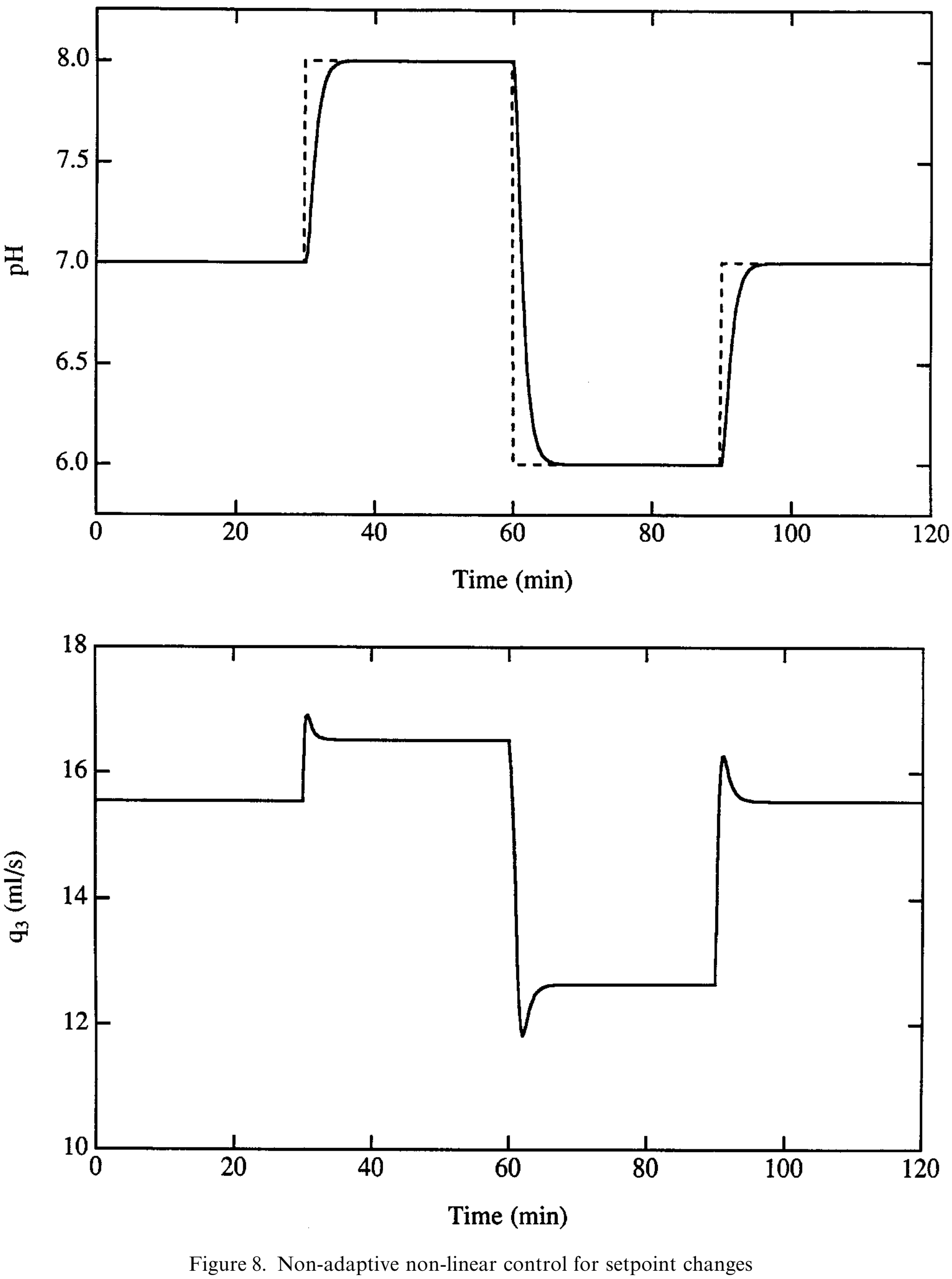

Figure 8. Non-adaptive non-linear control for setpoint changes

4.2. Direct adaptive non-linear control

Sastry and Isidori[36] have proposed a direct adaptive control strategy based on input–output linearization for non-linear systems with unknown, constant parameters. The approach yields asymptotic setpoint tracking and closed-loop stability if the zero dynamics are exponentially

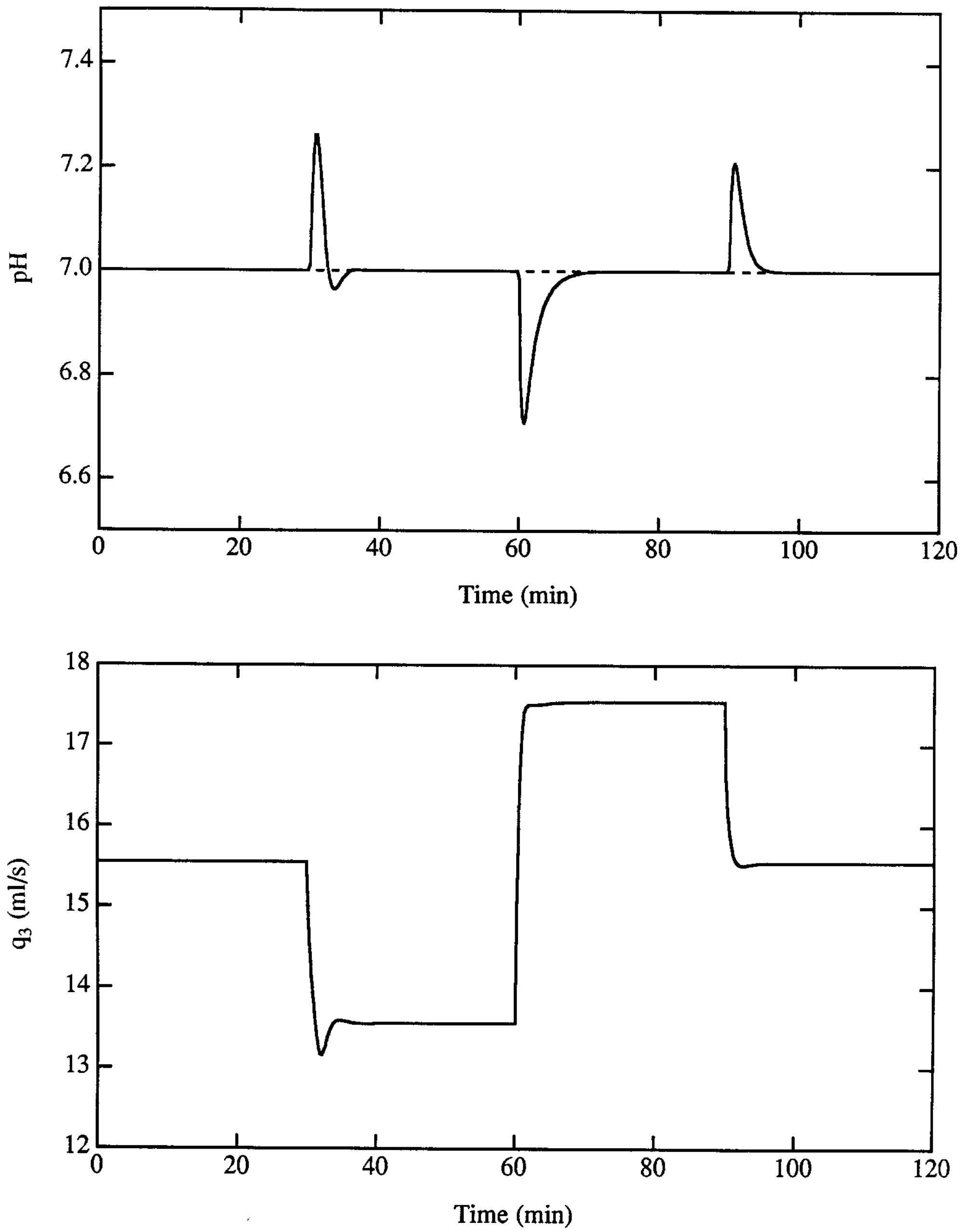

Figure 9. Non-adaptive non-linear control for acid flow rate disturbances

stable and Lipschitz continuous. Following their design procedure, (20) and (25) are combined to yield the closed-loop relation

$$\dot{y} + 2\varepsilon^{-1} y + \varepsilon^{-2} \int_0^t (y - y_{\mathrm{sp}})\mathrm{d}\tau = w(x, y)\,\Phi \tag{27}$$

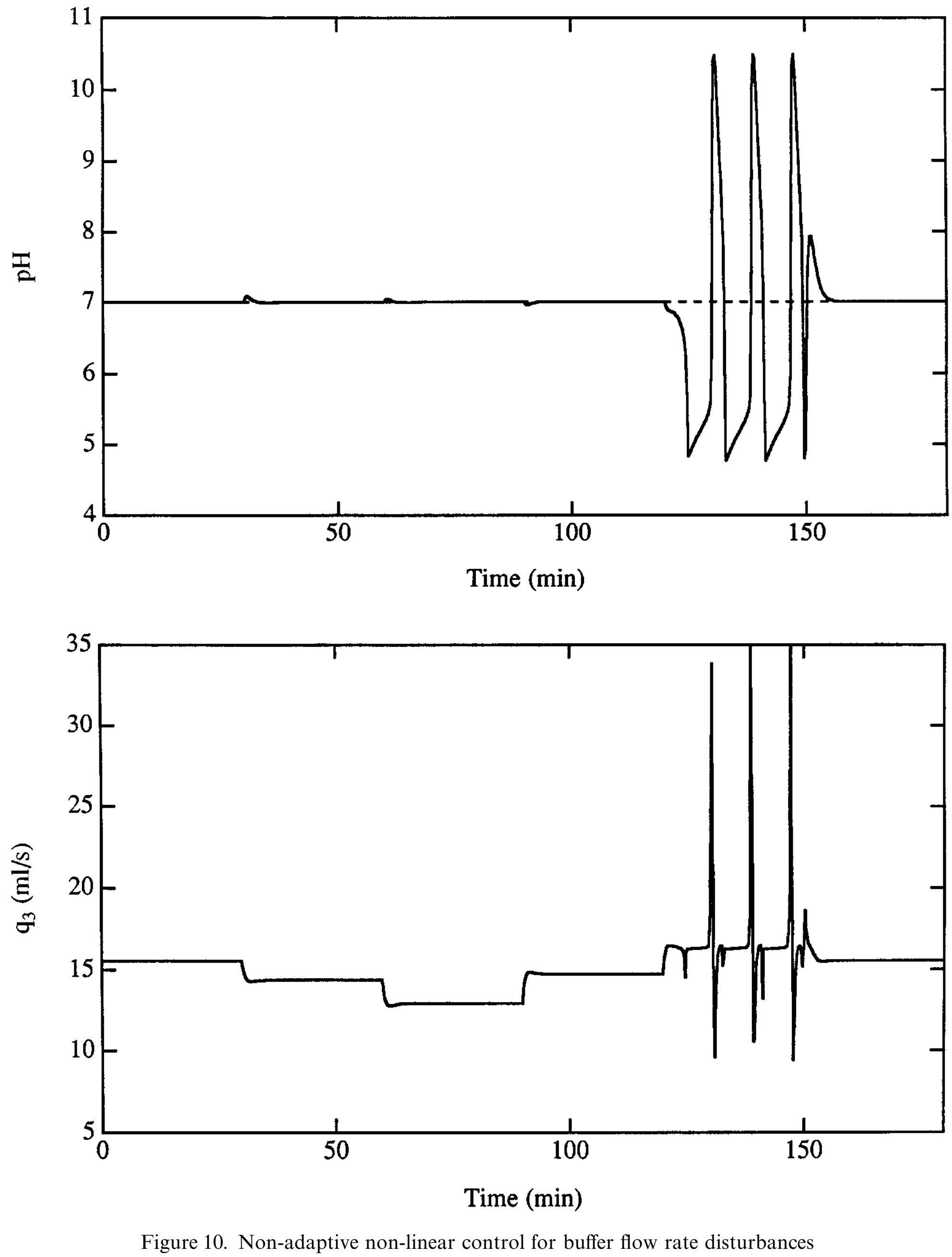

Figure 10. Non-adaptive non-linear control for buffer flow rate disturbances

where the regressor $w(x,y) = -c_y^{-1} c_{xP}$ and the parameter error $\Phi = d - \hat{d}$. The unknown parameter is estimated using an unnormalized gradient update law

$$\dot{\hat{d}} = e_1 w(x,y) = -(y - y_{\text{sp}}) c_y^{-1} c_{xP} \tag{28}$$

where the tracking error $e_1 = y - y_{\text{sp}}$.

We consider two modifications of the parameter estimator (28). First a normalized least squares update law with covariance resetting[37,38] is employed to provide faster parameter convergence. In addition, a modified tracking error is defined for the reason discussed below. Note that the update law (28) has the undesirable property that the estimated parameter may change if there is no actual parameter error. For example, consider a setpoint change when $\hat{d} = \text{d}$. Initially $y \neq y_{\text{sp}}$ and therefore $\hat{d}$ is modified as in (28). An alternative approach is to define the tracking error as the difference between the actual output and the desired output (26):

$$e_2(s) = y(s) - \frac{1}{(\varepsilon s + 1)^2} y_{\text{sp}}(s) \tag{29}$$

These modifications yield the parameter estimation scheme

$$\dot{\hat{d}} = \frac{Pwe_2}{1 + \text{Pw}^2}, \qquad \dot{P} = -\frac{P^2 w^2}{1 + Pw^2} \tag{30}$$

The covariance resetting algorithm is $P(0) = P(t_r) = 25$, where $t_r = \{t \,|\, |e_2| \geqslant 0{\cdot}025\}$. This parameter estimator is combined with the control law (25) to form the modified direct adaptive non-linear controller.

The undesirable setpoint tracking behaviour of the unmodified direct adaptive controller based on the error e_1 is displayed in Figure 11. In this case the adaptive controller is initialized with the exact value of the buffer flow rate ($\hat{d} = 0{\cdot}55$ ml s^{-1}) and a normalized least squares update law with covariance resetting is employed. Excellent tracking is obtained for the first and third setpoint changes, but the response is extremely oscillatory for the second change. This behaviour occurs because the estimator cannot recover from the covariance reset which occurs as a result of e_1 exceeding the tolerance. The tolerance cannot be increased to avoid covariance resetting without destroying the performance of the controller for other buffer flow rate disturbances. Similar behaviour is obtained when the unnormalized gradient update law (28) is used.

Significantly improved tracking performance can be obtained by employing the modified tracking error e_2 in (29). In this case the adaptive controller provides rapid setpoint tracking without oscillations as shown in Figure 12. The estimated parameter is essentially unaffected by the setpoint changes, because the tracking error e_2 remains well below the tolerance. Note that the pH responses and control moves are very similar to those produced by the non-adaptive controller (Figure 8).

The regulatory performance of the direct adaptive controller for the unmeasured buffer flow rate disturbances in Figure 5 is shown in Figure 13. In this test the setpoint is constant and there is no reason to discriminate between the unmodified and modified forms of the controller. The adaptive controller provides superior disturbance rejection as compared with the non-adaptive controller (Figure 10) when $q_2 \to 0$ ml s^{-1}. However, when $q_2 \to 0{\cdot}55$ ml s^{-1}, the adaptive controller produces an oscillatory pH response. The controller cannot be retuned to improve this behaviour without significant degradation of the response when $q_2 \to 0$ ml s^{-1}. Another disadvantage of the direct controller is that the estimated value of q_2 does not asymptotically converge to the true value because of the integral action in the control law (25). This behaviour is undesirable, because the estimated parameter can be used to generate estimates of the reaction invariants.[31] The direct adaptive controller yields a faster but more oscillatory pH response (not shown) for unmeasured acid flow rate disturbances as compared with the non-adaptive controller in Figure 9.[31]

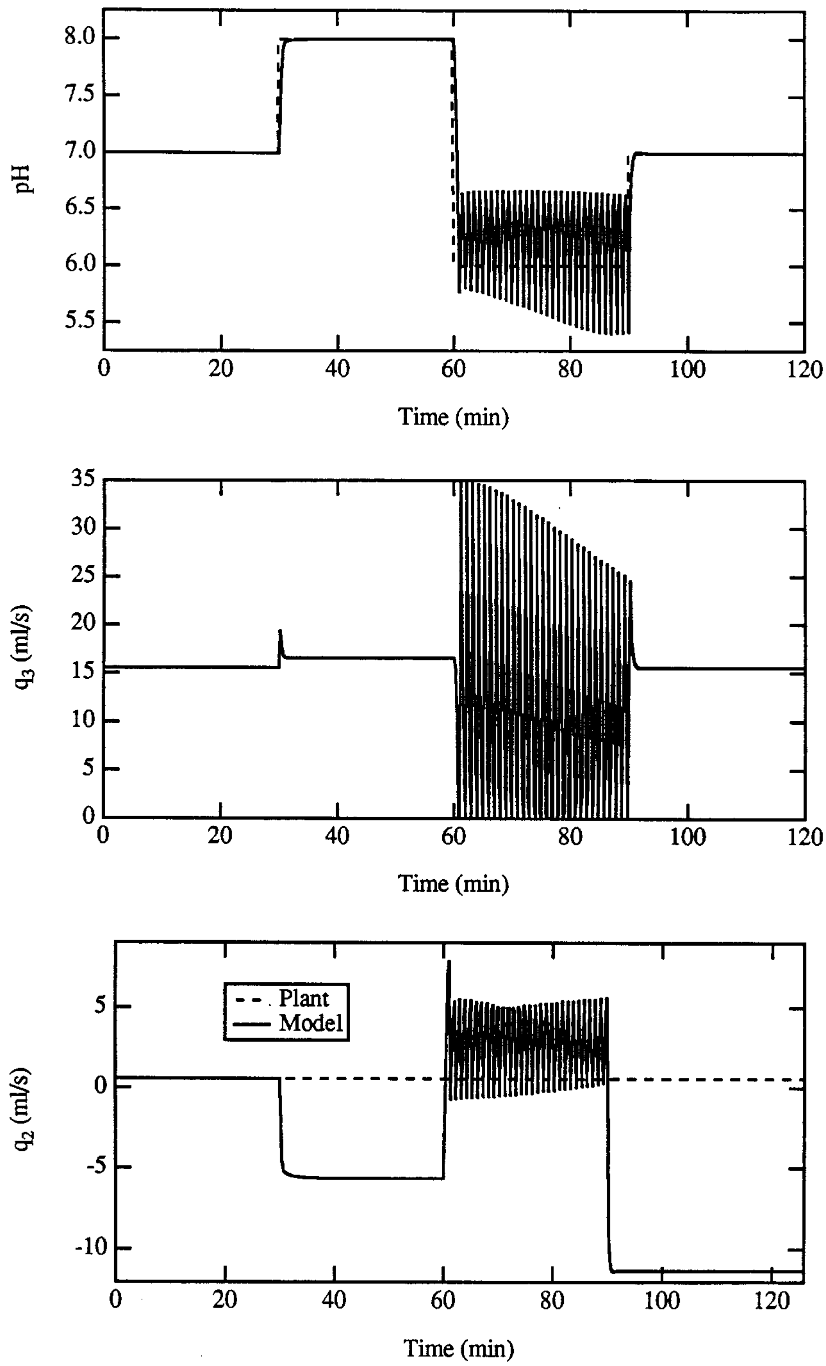

Figure 11. Direct adaptive non-linear control for setpoint changes

Figure 14 shows the effect of sampling on the direct adaptive controller. In this test a sampling period $\Delta t = 5$ s is employed for the buffer flow rate disturbances in Figure 4. The first three disturbances are rejected very effectively, but the system is unstable for the more demanding

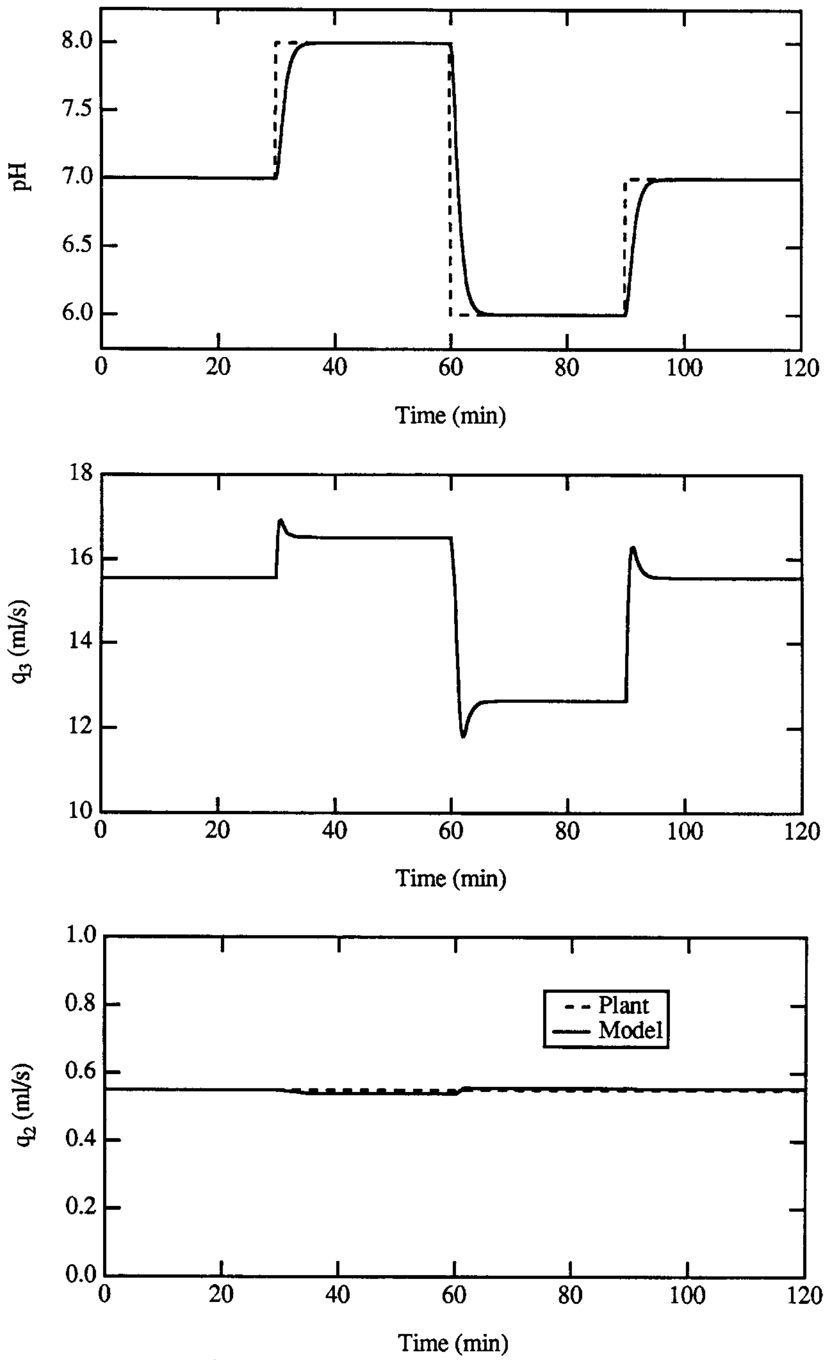

Figure 12. Modified direct adaptive non-linear control for setpoint changes

change when $q_2 \rightarrow 0$ ml s^{-1}. Note that the estimated buffer flow rate is exceptionally poor for this disturbance. Because of the poor parameter convergence properties and high sensitivity to sampling, the direct adaptive non-linear controller is not suitable for experimental implementation.[31]

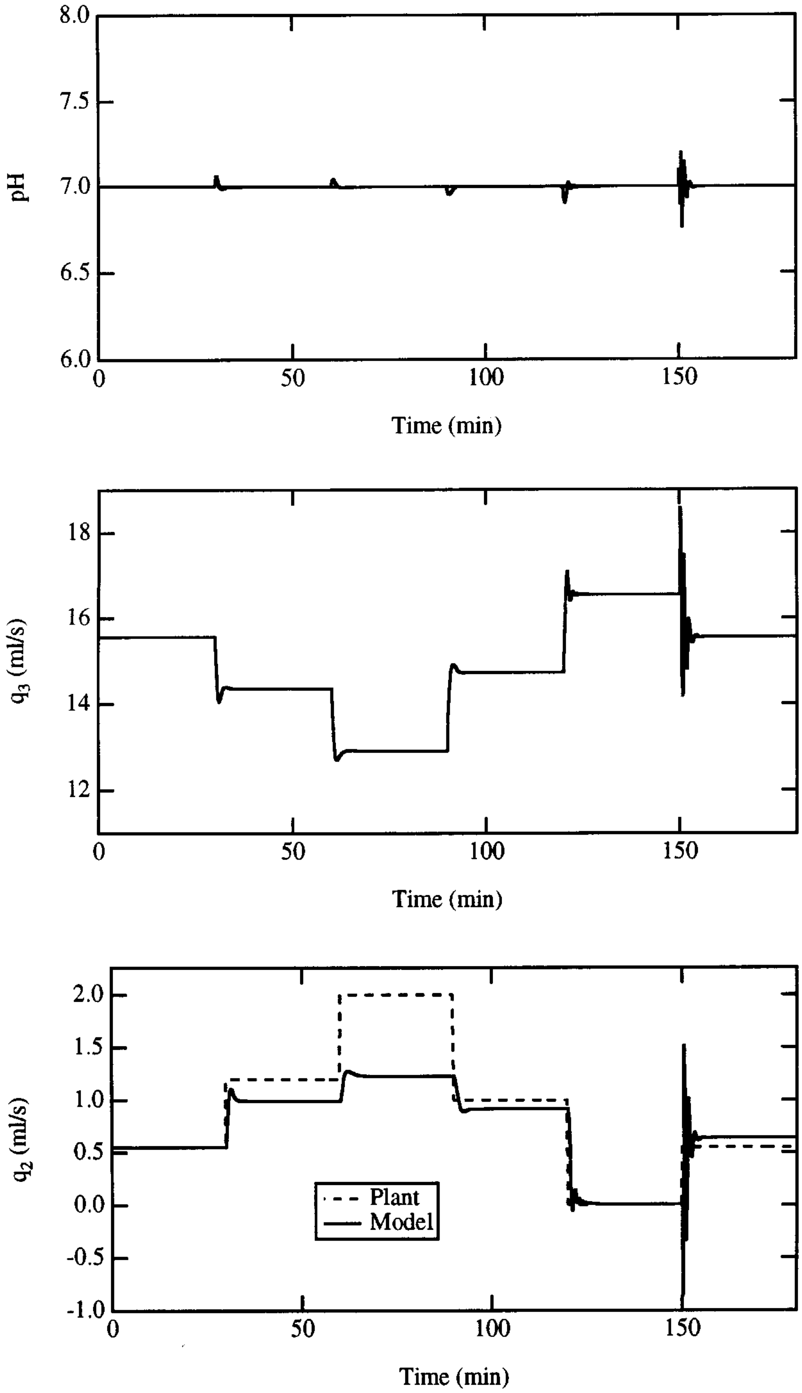

Figure 13. Direct adaptive non-linear control for buffer flow rate disturbances

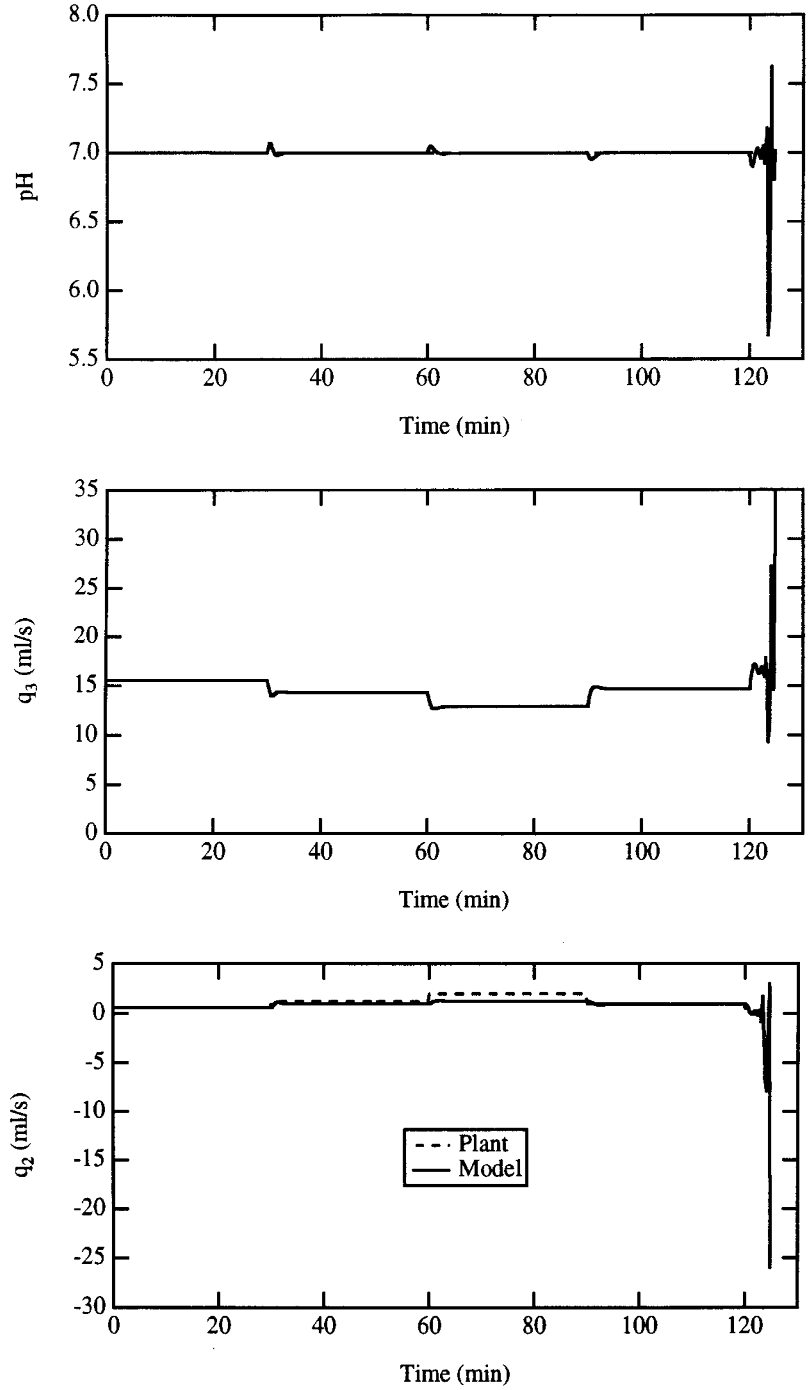

Figure 14. Direct adaptive non-linear control with $\Delta t = 5$ s for buffer flow rate disturbances

4.3. Indirect adaptive control based on a filtered regressor identifier

Teel *et al.*[39] have developed an indirect adaptive control strategy based on a filtered regressor identifier for linearly parametrized non-linear systems. The identifier has the following form for the pH neutralization model:

$$e_f \dot{W} = -W + f + gu + p\hat{d}, \qquad W(0) = 0 \tag{31}$$

$$e_f \dot{W}_0 = -W_0 + x, \qquad W_0(0) = x \tag{32}$$

where W and W_0 represent filtered estimates of $\dot{x}$ and x respectively and e_f is the time constant of the filters. An estimate of the state vector can be constructed from the filtered values: $\hat{x} = e_f W + W_0$. The parameter estimation is based on the error between the estimated and actual state variables :

$$e_3 = \frac{1}{e_f}(\hat{x} - x) \tag{33}$$

Consequently, this estimation scheme cannot be modified for the output feedback case where the reaction invariants are unmeasured.

A normalized least square algorithm can be employed for parameter estimation:

$$\dot{\hat{d}} = -\frac{Pp^{\mathrm{T}}e_3}{1 + Pp^{\mathrm{T}}p}, \qquad \dot{P} = -\frac{P^2 p^{\mathrm{T}} p}{1 + Pp^{\mathrm{T}}p} \tag{34}$$

where the vector p is defined as in (18). The covariance resetting algorithm is $P(0) = \mathrm{P}(t_r) = 3{\cdot}5 \times 10^8$, where

$$t_r = \{t \,|\, \frac{\|e_3\|}{\|x\|} \geqslant 0{\cdot}025\} \tag{35}$$

The filter time constant was chosen as $e_f = 0{\cdot}1$ min by trial and error. The parameter estimator is combined with the input–output linearizing control law (25) to form the indirect adaptive non-linear controller. This controller will be referred to as 'indirect adaptive controller #1' to distinguish it from the alternative indirect approach discussed in the next subsection. Asymptotic tracking and closed-loop stability are ensured only if the non-linear system satisfies restrictive growth conditions[39] which are difficult to verify for the pH neutralization model.

The regulatory performance of indirect adaptive non-linear controller #1 for the buffer flow rate disturbances in Figure 4 is shown in Figure 15. The controller provides excellent pH control for a wide range of buffering conditions as well as asymptotic tracking of the buffer flow rate and reaction invariants (not shown). Note that the indirect controller yields much smoother pH responses and control moves than the direct adaptive controller (Figure 13) for the last two disturbances. Although not shown, the performance of the indirect controller for setpoint changes and unmeasured acid flow rate disturbances is very similar to that of the non-adaptive controller (Figures 8 and 9). As compared with the direct controller, the indirect controller yields slower pH responses but much less aggressive control moves for acid flow rate changes.

The effect of sampling on indirect adaptive controller #1 is shown in Figure 16. The sampling period was increased to $\Delta t = 15$ s and the controller was subjected to the buffer flow rate disturbances in Figure 4. The pH deviations are small and the control moves are acceptable,

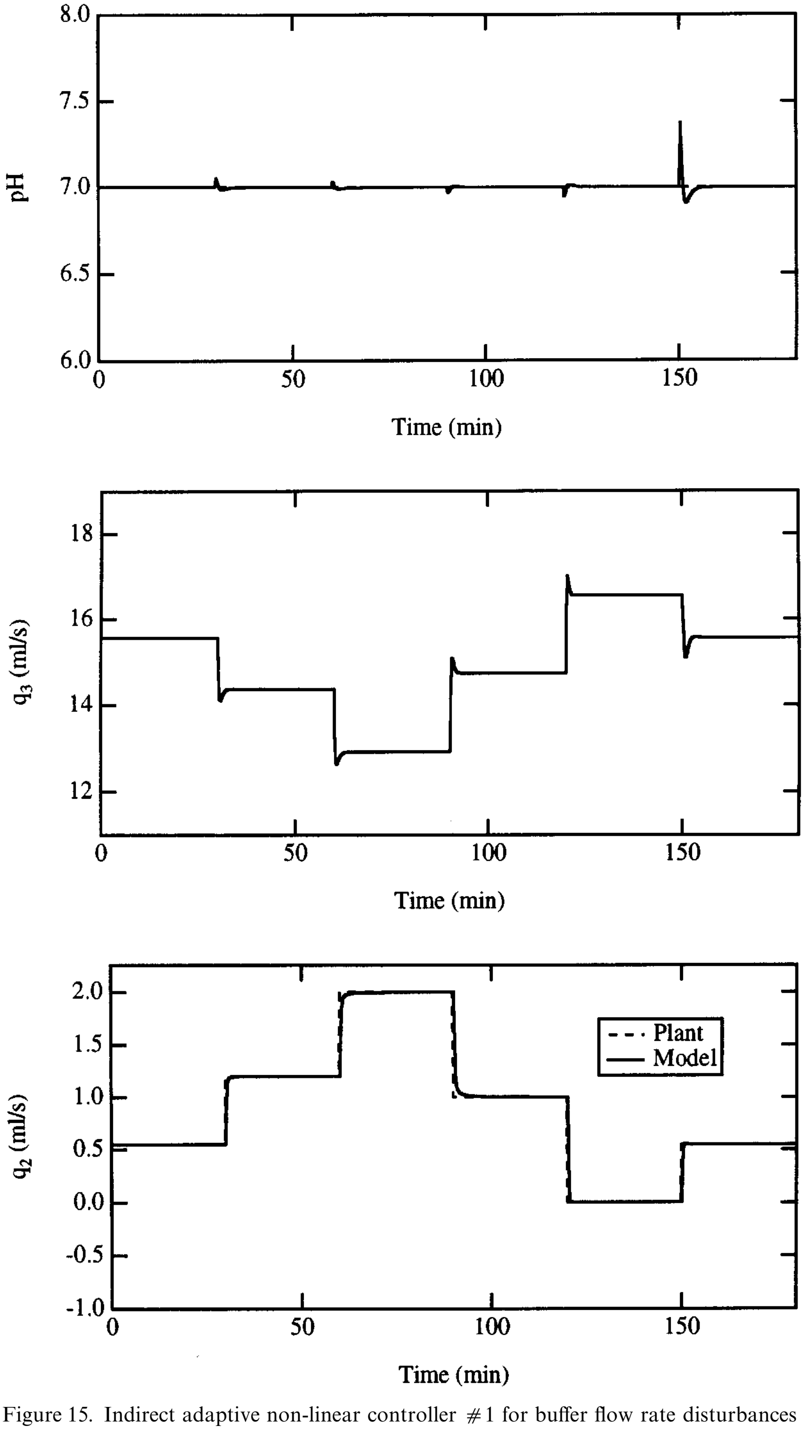

Figure 15. Indirect adaptive non-linear controller #1 for buffer flow rate disturbances

although more vigorous than in the case where $\Delta t = 1$ s (Figure 15). Less aggressive control moves can be obtained by increasing the closed-loop time constant ε. Excellent tracking of the buffer flow rate is also obtained. Note that the indirect controller provides superior performance

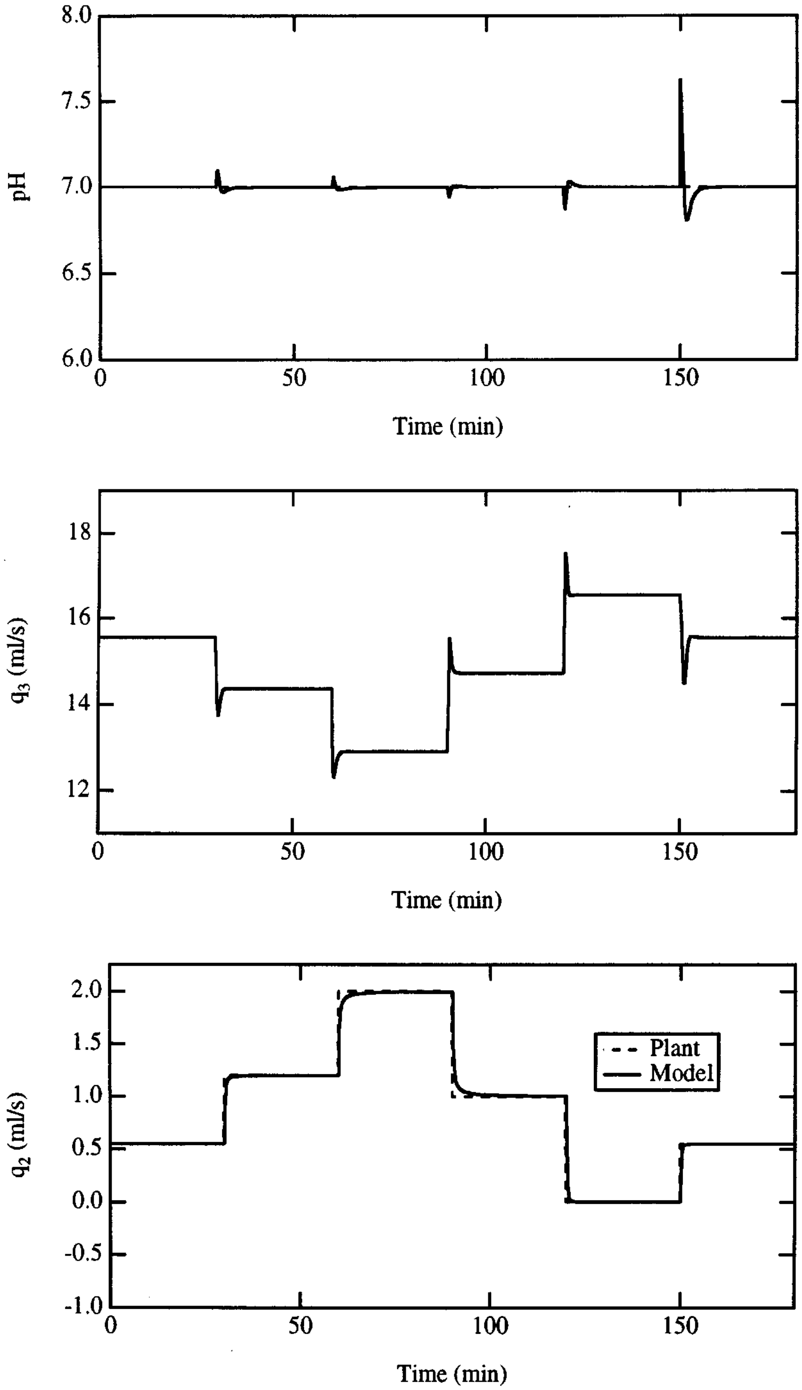

Figure 16. Indirect adaptive non-linear controller #1 with $\Delta t = 15$ s for buffer flow rate disturbances

to the direct controller when $\Delta t = 5$ s (Figure 14). However, indirect controller #1 cannot be implemented, because the parameter estimation scheme knowledge of the reaction invariants, which are not available in practice.

4.4. Indirect adaptive control based on a discretized error equation.

We now present an alternative adaptive non-linear control strategy which addresses the shortcomings of the direct and indirect adaptive controllers described in Sections 4.2 and 4.3 respectively. A discrete-time formulation is employed to facilitate experimental studies in which the sampling period $\Delta t = 15$ s.[40] The parameter estimator is designed as follows. First the time derivative of y in (20) is discretized using a central difference approximation which preserves the linear parametrization. The resulting expression is

$$y_k = y_{k-2} - \Delta t\, c_y^{-1}(x_{k-1}, y_{k-1})\, c_x(x_{k-1})\, [f(x_{k-1}) + g(x_{k-1})u_{k-1} + p(x_{k-1})\, d_{k-1}] \tag{36}$$

where the subscript k denotes the current sampling instant. The estimation equation follows directly from (36):

$$v_k = \eta_k\, d_{k-1} \tag{37}$$

where

$$v_k = \Delta t\, c_y^{-1}(x_{k-1}, y_{k-1})\, c_x(x_{k-1})\, [f(x_{k-1}) + g(x_{k-1})u_{k-1}] + y_k - y_{k-2} \tag{38}$$

$$\eta_k = -\Delta t\, c_y^{-1}(x_{k-1}, y_{k-1})\, c_x(x_{k-1})\, p(x_{k-1}) \tag{39}$$

All the information needed to compute v_k is available, since the reaction invariants are assumed to be measured. Thus the estimation error is defined as

$$e_{4k} = v_k - \eta_k\, \hat{d}_{k-1} \tag{40}$$

The buffer flow rate is updated using a normalized least squares estimator

$$\hat{d}_k = \hat{d}_{k-1} + \frac{P_{k-2}\eta_k e_{4k}}{1 + P_{k-2}\eta_k^2} \tag{41}$$

$$P_{k-1} = P_{k-2} - \frac{P_{k-2}^2 \eta_k^2}{1 + P_{k-2}\eta_k^2} \tag{42}$$

The covariance resetting algorithm is $P(0) = P(k_r) = 1 \times 10^4$, where $k_r = \{k \mid |e_{4k}| \geqslant 2{\cdot}5 \times 10^{-3}\}$. The parameter estimator is combined with the control law (25) to form the adaptive non-linear controller, which will be referred to as 'indirect adaptive controller #2'.

The regulatory performance of indirect adaptive controller #2 for the buffer flow rate disturbances in Figure 4 is shown in Figure 17. The pH response is superior to that produced by the PI (Figure 6), non-adaptive (Figure 10), direct adaptive (Figure 13) and indirect adaptive #1 (Figure 15) controllers. The parameter tracking performance of indirect controller #2 is vastly superior to that of the direct controller (Figure 13) and very similar to that obtained with the indirect controller #1 (Figure 15). Figure 18 shows that indirect controller #2 provides significantly improved pH control for unmeasured acid flow rate disturbances as compared with the non-adaptive controller (Figure 9) despite generating inaccurate estimates of the buffer flow rate. Similar results are obtained when indirect controller #2 is compared with the PID, direct adaptive and indirect adaptive #2 controllers.[31] The setpoint response of indirect controller #2 (not shown) is almost identical with that produced by the non-adaptive controller shown (Figure 8).

The effect of sampling on indirect controller #2 is shown in Figure 19. In this test the sampling period has been increased from $\Delta t = 1$ s to the nominal experimental value $\Delta t = 15$ s and the

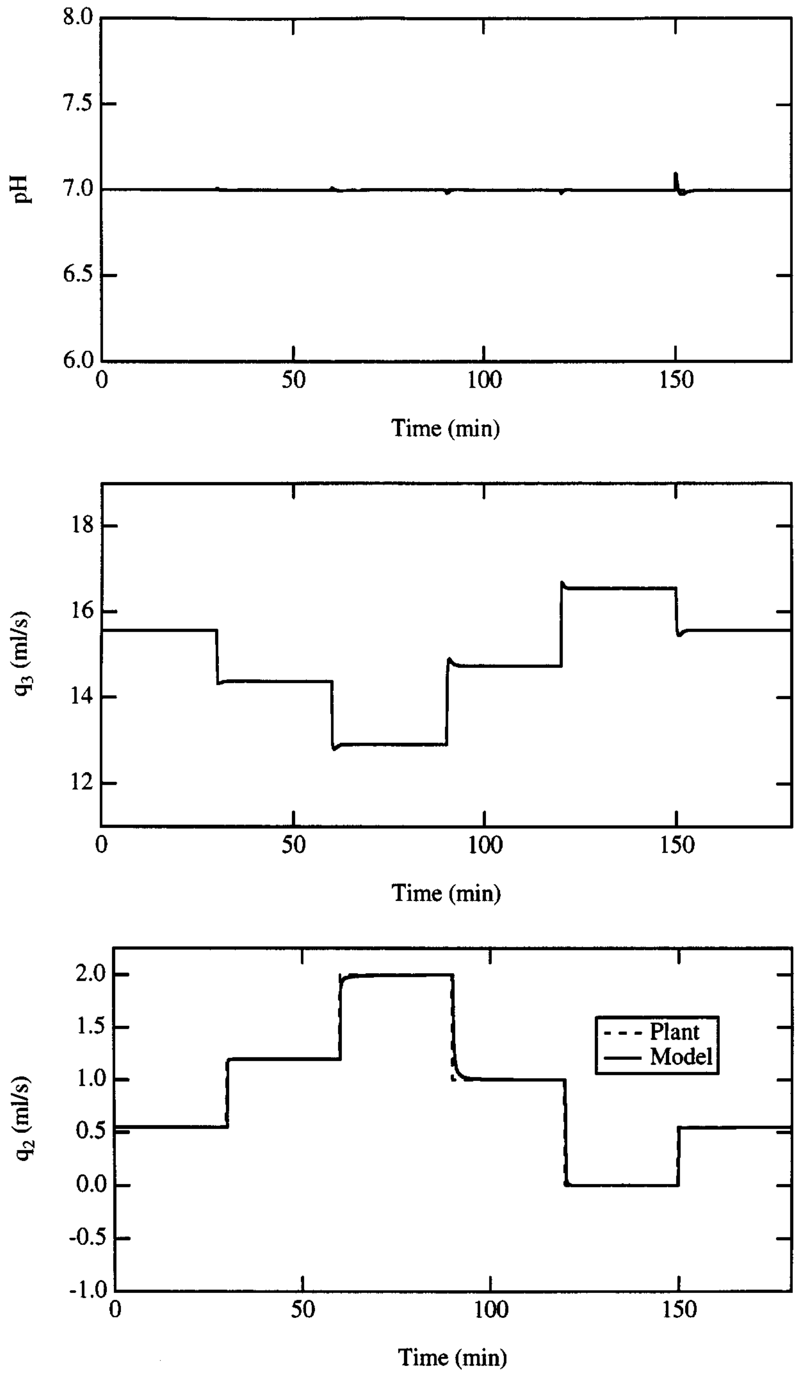

Figure 17. Indirect adaptive non-linear controller #2 for buffer flow rate disturbances

controller is subjected to the buffer flow rate disturbances in Figure 4. Indirect controller #2 provides improved pH regulation as compared with the direct controller (Figure 14) and indirect controller #1 (Figure 16). As expected, the closed-loop performance is degraded as compared

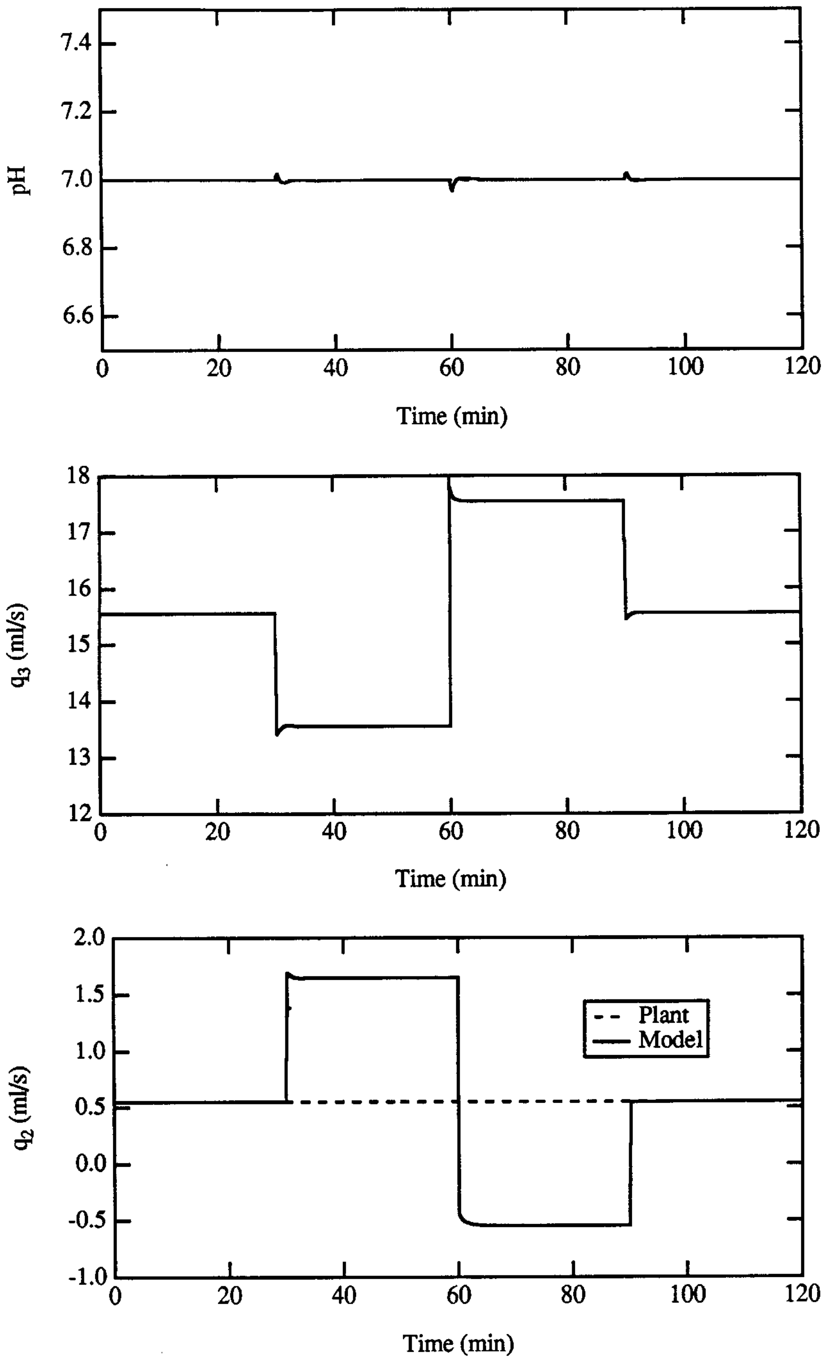

Figure 18. Indirect adaptive non-linear controller #2 for acid flow rate disturbances

with the case where $\Delta t = 1$ s (Figure 17). The increased sampling period results in larger pH deviations from the setpoint, more vigorous control moves and slightly poorer parameter tracking. Note that less aggressive control moves can be obtained by increasing the closed-loop time constant ε.

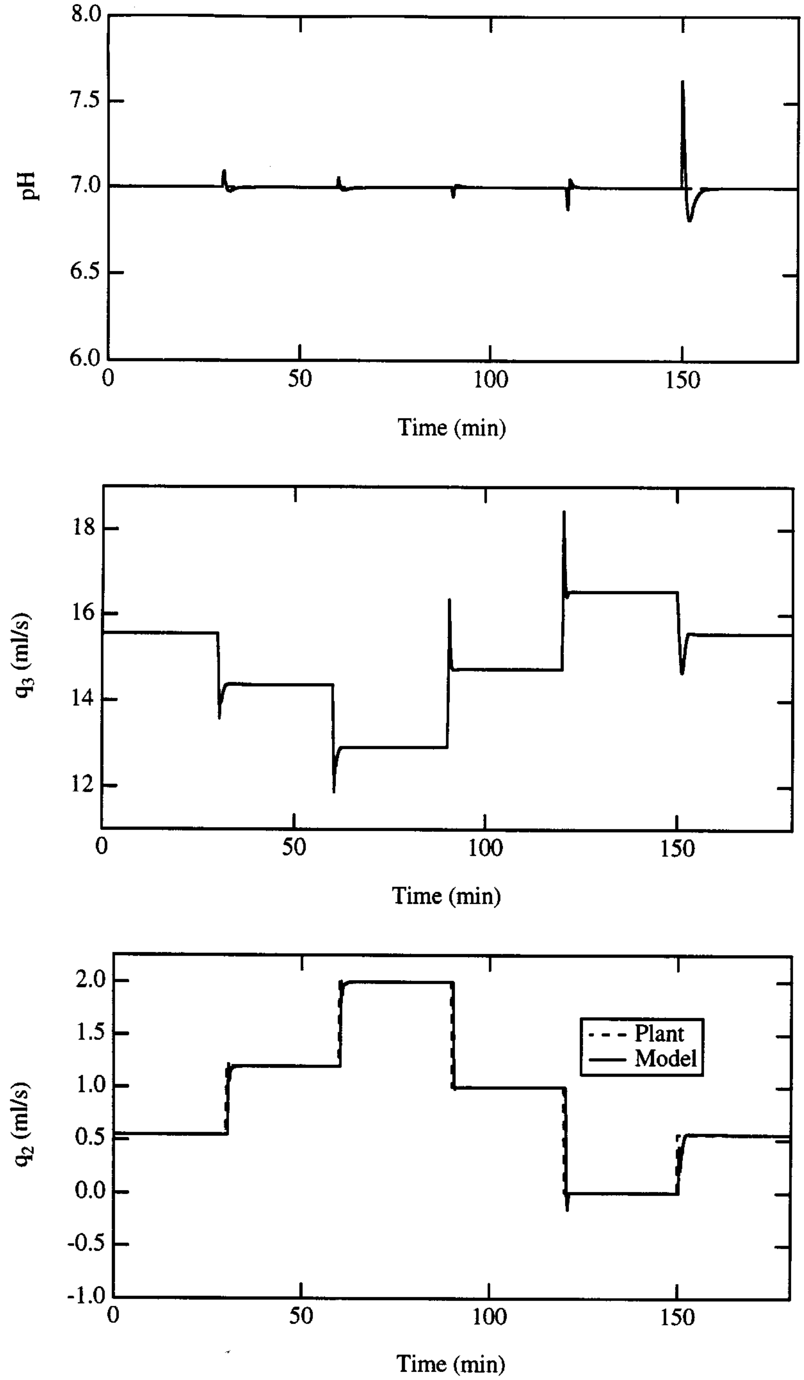

Figure 19. Indirect adaptive non-linear controller #2 with $\Delta t = 15$ s for buffer flow rate disturbances

These simulation results demonstrate that the proposed indirect adaptive control strategy provides excellent setpoint tracking and disturbance rejection, asymptotic parameter tracking and robustness to sampling. Despite the lack of closed-loop stability guarantees, the proposed strategy provides superior performance as compared with the alternative adaptive schemes described in Sections 4.2 and 4.3. Moreover, the proposed technique can be modified for experimental applications in which the reaction invariants cannot be measured. An output feedback version of the indirect control strategy has been successfully applied to the UCSB bench-scale pH neutralization system.[40]

5. CONCLUSIONS

Three adaptive non-linear control strategies have been developed for the UCSB pH neutralization system using a reaction invariant model. For simplicity the reaction invariants are assumed to be available for feedback. The adaptive controllers are designed by combining an input–output linearizing controller with different non-linear parameters estimators which account for unmeasured buffering changes. Simulation results demonstrate that a novel indirect strategy provides superior servo and regulatory performance as compared with the direct scheme of Sastry and Isidori[36] and the indirect scheme of Teel *et al.*[39] Moreover, the proposed technique is suitable for on-line implementation where the reaction invariants must be estimated and sampling is required.

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