ON UTILISING STRUCTURAL INFORMATION FOR ADAPTIVE CONTROL OF A PH NEUTRALISATION PROCESS

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Abstract

Control of the pH level is of vital importance in many industrial applications. However, pH control has only met with limited success. A stumbling block is the severe non-linearity of titration processes. One control strategy that have been employed to overcome the process non-linearity exploits the knowledge that certain pH processes can be casted in the Wiener model structure. In practice, it is very likely that the process characteristics will be affected by the presence of unknown buffers. This paper aims at examining whether there are merits in using structural information to design the architecture of adaptive controllers in situations where the knowledge may be inaccurate due to changing buffering conditions. The main finding of this work is that a “black box” controller is better able to adapt to the changing dynamics caused by the introduction of an unknown buffer.

1 Introduction

pH control is a typical requirement found in industries such as wastewater treatment, pharmaceutical, biotechnology, and chemical processing. It is a challenging problem because of the severe non-linearity of the titration process, and a large variety of control schemes for pH control have been proposed. Increasingly, neural networks and fuzzy logic techniques [1, 2] are being utilised. This trend is mainly fuelled by the fact that neural and fuzzy systems have universal approximation capabilities. It is, therefore, not surprising that most control schemes are constructed by treating the nonlinear pH process as a non-linear “black box” model [3]. Despite the wealth of control schemes that have been employed, only limited success has been achieved. One reason is that the exact composition of the reagents in the many practical processes, like the treatment of wastewater, is unknown. As the introduction of unknown buffers into a pH process can change the nominal plant dynamics significantly, an ability to adapt to the prevailing conditions is a pre-requisite for good control of an industrial pH process.

In this paper, an adaptive neurofuzzy controller is used to control a pH neutralisation process. Since traditional pH control strategies generally try to embed information about the process titration curve into the controller, another objective of this work is to examine whether there are merits in using *a prior* structural information to design the architecture of adaptive neurofuzzy controllers in situations where the knowledge may be inaccurate due to changing buffering conditions. The rest of the paper is organised as follows : first, the mechanics of the pH process in a Continuously Stirred Tank Reactor (CSTR) are described. Next, the adaptive neurofuzzy control scheme is presented. Simulation results are then used as the basis for analysing the benefits of incorporating structural knowledge into the control structure. Finally, Section 5 concludes the paper.

2 The pH Process

The pH process considered in this paper is the neutralisation of two monoprotic reagents : a weak acid (acetic acid, CH_3COOH, that has a concentration of 0.05M) and a strong base (sodium hydroxide, $NaOH$, whose concentration is 0.1M). The following chemical reactions occur when CH_3COOH is mixed with $NaOH$:

$$\begin{aligned} H_2O &\Leftrightarrow H^+ + OH^- && (1a) \\ CH_3COOH &\Leftrightarrow H^+ + CH_3COO^- && (1b) \\ NaOH &\rightarrow Na^+ + OH^- && (1c) \end{aligned}$$

According to the electro-neutrality condition, the nett sum of the ionic charges must be zero. Therefore,

$$[Na^+] + [H^+] = [CH_3COO^-] + [OH^-] \qquad (2)$$

where $[X]$ denotes the concentration of X ion. Defining $x_a = [CH_3COO^-] + [CH_3COOH]$ as the weak acid ionic concentration and $x_b = [Na^+]$ as the base ionic concentration, the neutralisation equation for the titration process is

$$\begin{aligned} &[H^+]^3 + [H^+]^2(K_a + x_b) + \\ &\quad [H^+]K_a(x_b - x_a) - K_w - K_wK_a = 0 \qquad (3) \end{aligned}$$

where $K_a = \frac{[CH_3COOH^-][H^+]}{[CH_3COOH]} = 10^{-4.75}$ is the acid dissociation constant for acetic acid at 25^oC, and $K_w = \frac{[H^+][OH^-]}{[H_20]} = 10^{-14}$ is the ionic product at 25^oC. Letting $pH = -\log_{10}[H^+]$ and $pKa = -\log_{10}[K_a]$, the titration curve may be defined as

$$x_b + 10^{-pH} - 10^{pH-14} - \frac{x_a}{1 + 10^{pK_a - pH}} = 0 \qquad (4)$$

The neutralisation process takes place in a CSTR. Assuming that mixing is perfect, the mixing dynamics can be described as [4]

$$V\frac{dx_a}{dt} = F_aC_a - (F_a + F_b)x_a \qquad (5a)$$

$$V\frac{dx_b}{dt} = F_bC_b - (F_a + F_b)x_b \qquad (5b)$$

F_a is the flow rate of the influent stream (CH_3COOH), F_b is the flow rate of the titrating stream ($NaOH$), C_a is the concentration of the influent stream, C_b is the concentration of the titrating stream, x_a is the ionic concentration of the acid solution (mol/litre), x_b is the ionic concentration of the base solution (mol/litre), and V is the volume of the mixture in the CSTR (2 litres).

The theoretical CSTR mixing dynamics, defined in Equation (5), is bilinear. In practice, the concentration of the reagents used in the titrating stream can generally be chosen such that the acid flowrate is much larger than the base flowrate i.e. $F_a >> F_b$. This implies that the CSTR dynamics may be approximated by the linear differential equations shown below if C_a is selected carefully :

$$V\frac{dx_a}{dt} \approx F_a(C_a - x_a) \qquad (6a)$$

$$V\frac{dx_b}{dt} \approx F_bC_b - F_ax_b \qquad (6b)$$

To sum up, the equations indicate that the process of neutralising a weak acid with a strong base in a CSTR may be approximated by the Wiener-type non-linear model shown in Figure 1. This structural information can be exploited to simplify the control problem. A common approach is to attempt to cancel the system non-linearity by cascading an inverse model of the neutralisation relationship to the process. The performance of systems that adopt the Wiener-model controller structure often hinges on how well the non-linearity is cancelled. When the process dynamics changes continuously due to buffering variations or flowrate changes, the inverse model may become inaccurate, and thus causing the control performance to worsen. The goal of the work described herein is to examine if there are advantages in employing the Wiener-model control structure when disturbances lead to a deterioration in the accuracy of the inverse model. Before presenting the results of the study, the adaptive neurofuzzy control scheme is described in the next section.

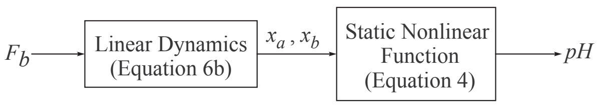

Figure 1: The Wiener non-linear model

3 The Adaptive Control Strategy

Figure 2 shows the block diagram of the adaptive neurofuzzy controller that utilises the feedback error learning strategy to perform on-line training [5]. There are four main components in the control scheme : (i) a neurofuzzy feedforward controller, (ii) an on-line identification mechanism (iii) a proportional controller, and (iv) a reference model. Adaptive control is attained by determining the parameters of the neurofuzzy feedforward controller on-line such that it approximates the inverse input-output mapping of the plant. As the adaptive controller does not make use of any prior information about the pH process, it may be classified as a “black box” approach.

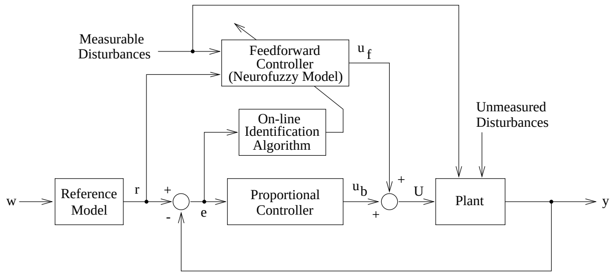

Figure 2: General structure of the control scheme

In order to train the neurofuzzy controller on-line, the input that should be applied to the plant for the process output to reach a desired state must be available. As this information is usually unknown *a priori*, an estimate is generated via the following equation:

$$\tilde{u}_f(t) = u_f(t - t_d) + \gamma e(t) \qquad (7)$$

where $\tilde{u}_f(t)$ is the estimate of the required control action at sampling instant t, $u_f(t - t_d)$ is the output of the feedforward controller t_d sampling instants earlier, t_d is the transportation delay expressed as a multiple of the sampling time and γ determines the proportion of the feedback error, $e(t) = r(t) - y(t)$ used to estimate the desired control action. Equation (7), known as the feedback error learning rule, is based on the observation that $e(t)$ may be non-zero if an erroneous control action was applied t_d sampling instants ago. Hence, the feedback error may be viewed as the modelling error and used to derive a new estimated of the required control action. Since the output of a neurofuzzy model is linear-in-the-parameters i.e. $u_f(t) = \mathbf{a}^T(t)\mathbf{w}(t)$ ($\mathbf{a}(t)$ is the transformed input vector and $\mathbf{w}(t)$ is the weights vector), the feedforward controller may then be updated by passing $\tilde{u}_f(t)$ to the Normalised Least-Mean-Square (NLMS) algorithm:

$$\mathbf{w}(t) = \mathbf{w}(t-1) + \frac{\delta \mathbf{a}(t)}{\mathbf{a}^T(t)\mathbf{a}(t)}\epsilon(t) \qquad (8)$$

$\epsilon(t)$ is the modelling error. In summary, the on-line learning mechanism comprises two interdependent optimisation algorithms : the feedback error learning strategy for determining the required control action and the NLMS algorithm for updating the parameters of the neurofuzzy model.

In practice, an exact inverse model is difficult, if not impossible, to derive so the feedforward controller will exhibit finite modelling errors. A proportional controller (k_p) is, therefore, included in the feedback path to compensate for modelling mismatches. Another essential component of the scheme is the reference model. It filters the step changes in the setpoints in order to provide a reference trajectory that may be followed by the plant given the physical constraints and plant dynamics.

4 Simulation Results

This section details the investigations into the differences in control performances, with and without the usage of the *a prior* information that a weak-acid strong-base neutralisation process may be modelled by a Wiener-type non-linear system. The study is conducted by using the control schemes to track transitions between different pH levels. The setpoint changes are smoothen by a first order reference model with a time constant of 20 seconds. Two tests were performed. The first test examines their performance under nominal conditions. In the second test, carbonic acid (H_2CO_3), a diprotic reagent with pK_a of 6.35 and 10.25 at 0.2M, is added to the pH plant according to the schedule shown in Table 1. In order to understand the changes that are brought about by the introduction of the buffer, the titration curves are illustrated in Figure 3 below. The plots clearly show that the buffer has a significant impact on the shape of the titration curve at high pH levels. This is because the molarity of the buffer used is quadruple that of the acetic acid. The nett result is that the quality of any a prior information used that is incorporated in the controller will degrade severely. To prevent the control performance from deteriorating, the controller has to learn to adapt to the prevailing neutralisation characteristics on-line.

Buffer flowrate, F_c (ml//min)	Time (min)
0	0-600 and 2400-3000
100	600-1200 and 1800-2400
200	1200-1800

Table 1: Buffer flowrate variation schedule

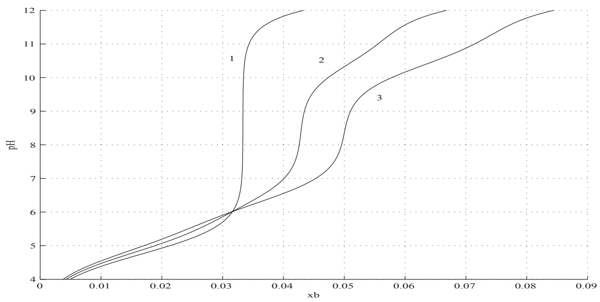

Figure 3: Titration relationship between x_b and pH under different buffer flowrates, F_c
(1) F_c=0, (2) F_c=100, (3) F_c=200 ml/min

4.1 Wiener-model controller

To begin the analysis, the structural information presented in Section 2 is used to derive the controller architecture shown in Figure 4. The static inverse titration model, h^{-1}, transforms the output pH value into an estimate of the base ionic concentration (x_b^*). pH control is then performed by using the adaptive neurofuzzy controller to provide the titrating flow rate, F_b, so that the difference between x_b^* and the reference base ionic concentration $x_{b,set}^*$ is minimised. Since the $F_b - x_b$ relationship is approximately linear (Equation 6), the control problem is, in theory, simpler.

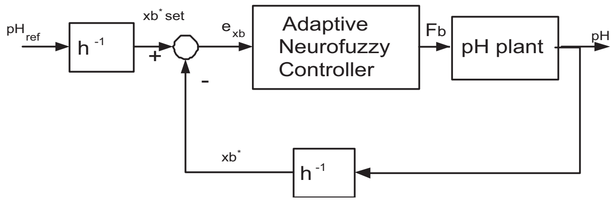

Figure 4: Structure of the Wiener-model controller

A B-spline network, with 13 second order B-splines spanning the input domain, was used to model the inverse neutralisation relationship. Input output data obtained from the nominal acid-base titration curve was used to identify the network parameters off-line. The resulting average modelling error (difference between the inverse model and the actual titration curve) is 0.0018%. Since h^{-1} only approximates the inverse titration curve, a zero feedback error, i.e. $e_{xb} = x_{b,set}^* - x_b^* = 0$, does not necessarily mean that the desired and reference pH are equal. To ensure that the feedback error learning rule actively tries to minimise $(pH_{ref} - pH)$, the difference between the reference pH value and the actual pH is used to estimate the required feedforward control action i.e. Equation (7) becomes $\tilde{u}_f(t) = u_f(t - t_d) + \gamma(pH_{ref} - pH)$. The parameters of the adaptive neurofuzzy controller are as follows : γ is 0.03, k_p is 0.18, the NLMS algorithm's update rate (δ) is 1 and sampling time is 5 seconds. $x_{b,set}^*$, the reference base ionic concentration, its rate of change ($\Delta x_{b,set}^*$), and x_b^*, the base ionic concentration derived from the static inverse model, were selected as the inputs of the neurofuzzy controller. The input domains were spanned by 5, 2, 2 triangular fuzzy sets respectively. All the elements in the weight vector of the neurofuzzy controller are arbitrarily initialised to 0.1.

Figure 5 shows the performance of the Wiener-model controller under nominal conditions. It shows that rapid convergence to the reference pH trajectory is obtained. While good tracking performance occurs in the mid pH range (7 to 11), the step responses at the bottom 6 to 7) and top (11 to 11.5) of the pH test range exhibit a mild overshoot and slightly sluggish behaviour respectively. Figure 6 displays the performance of the control scheme when the pH process is influenced by carbonic acid according to the schedule shown in Table 1. The performance of the control scheme degenerates upon the introduction of the buffer. This effect is more prominent in the higher pH levels, probably because of the larger changes to the titration curve in this region (See Figure 3). The results indicate that the adaptive neurofuzzy controller is unable to compensate for the deviations in the inverse neutralisation curve brought about by the addition of carbonic acid. It may be intuitively be argued that the use of erroneous *a prior* information caused the quality of the control to worsen. A natural extension is to try to modify the inverse titration model on-line.

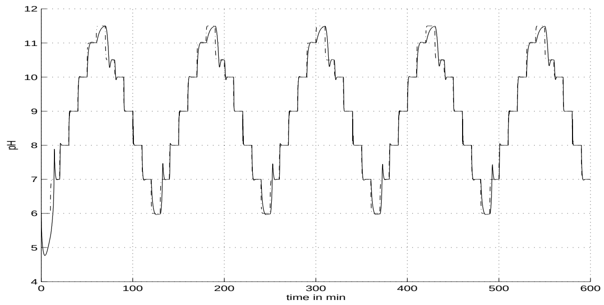

Figure 5: Performance of the Wiener-model controller under nominal conditions

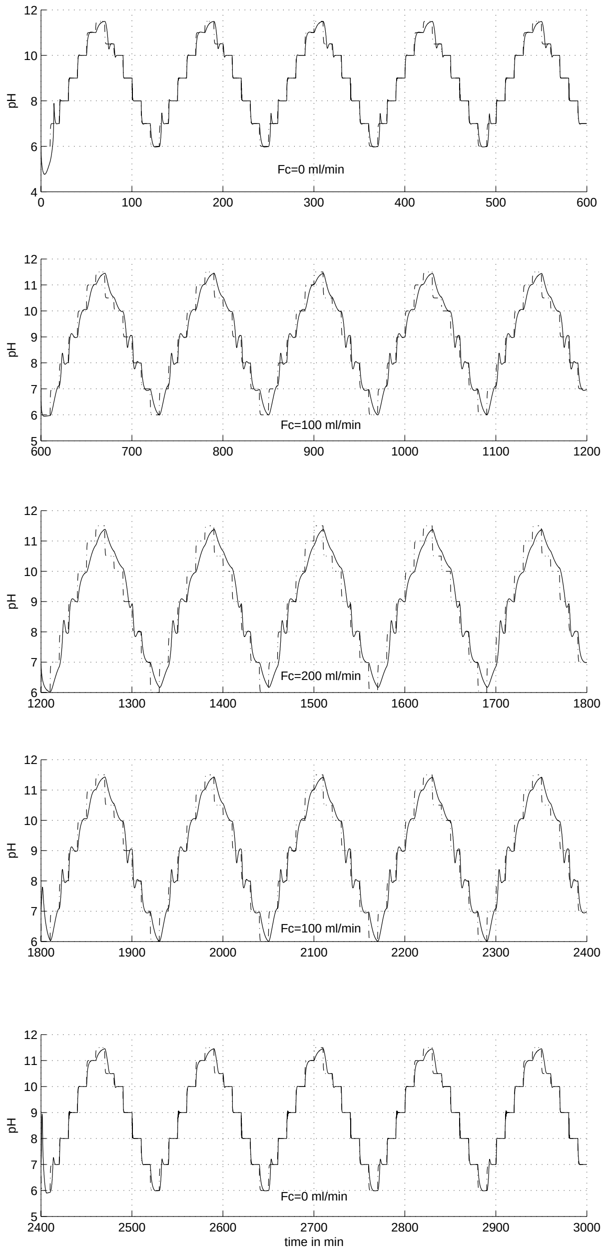

Figure 6: Performance of the Wiener-model controller when an unknown buffer is introduced

4.2 Adaptive Wiener-model Controller

To adapt the inverse neutralisation model on-line, the actual ionic concentrations of the various reagents must be known. As ion selective probes are expensive and the conversion rate is generally too slow for on-line use, the theoretical relationship defined in Equation (6) was used to estimate the actual ionic concentration corresponding to a pH value [7]. At each sampling instant, the estimated basic ionic concentration, together with the measured pH value, were then fed to a NLMS algorithm (learning rate, δ, is 0.75) to update inverse titration relationship (h^{-1}). In order to provide a common basis for comparison, the structure of the neurofuzzy feedforward controller was not changed. The proportional gain of the conventional controller (k_p), the learning rate for the feedback error learning scheme (γ) and the sampling time were chosen as 0.1, 0.05 and 1 seconds respectively.

The step responses obtained using the adaptive Wiener-model controller is shown in Figure 7. Compared with the results obtained using an inverse model that is not adapted on-line (Figure 5), better tracking performance was obtained. In particular, the step responses no longer overshoot the setpoint in the 6-7 pH range while the speed of response is faster at high pH values. Figure 8 shows the control responses when the pH plant is subjected to variations in the amount of buffering. Although the adaptive Wiener-model controller is able to better reject the undesirable effects of the unknown buffer, the control performance is still not very satisfactory. Following a change in the flowrate of carbonic acid from 100 ml/min to 0 ml/min, the pH value oscillates wildly when the setpoint is in the sensitive pH region. As several training cycles are needed to eliminate the oscillations, the adaptive Wiener-model controller will be of limited use in practice.

4.3 Adaptive neurofuzzy control : a "Black Box" approach

Since the performances of control schemes that exploit the Wiener-model representation may not be acceptable practically, the feasibility of employing the adaptive neurofuzzy controller to regulate the output pH directly is examined. The inputs to the neurofuzzy feedforward controller are selected as the reference pH level, $pH_{set}(k)$, its rate of change $\Delta pH_{set}(k)$, and the control action $U(k)$. Eight uniformly distributed triangular fuzzy sets partition the universe of discourse for the first input, $pH_{set}(k)$, while the input space for $\Delta pH_{set}(k)$ and $U(k)$ are partitioned by two fuzzy sets each. As there are large variations in the pH dynamics, it may be difficult for the adaptive neurofuzzy controller to learn at a appropriate rate using a common set of controller parameters. Hence, the controller parameters are scheduled according to the region in which the process is operating. When the reference pH levels are between 7 and 10, k_p and γ are 0.3628 and 0.0021 respectively. k_p and γ assume the values 2.5 and 0.1 respectively whenever the reference pH levels are between $6 - 7$ and $10 - 11.5$. The learning rate for the NLMS algorithm and

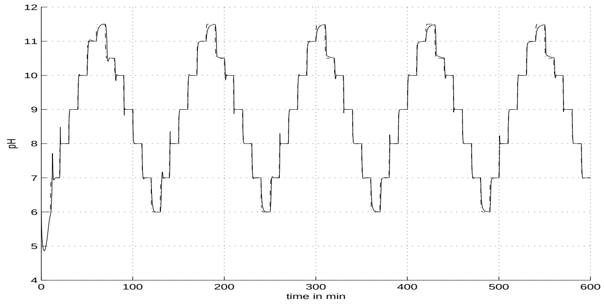

Figure 7: Performance of the adaptive Wiener-model controller under nominal conditions

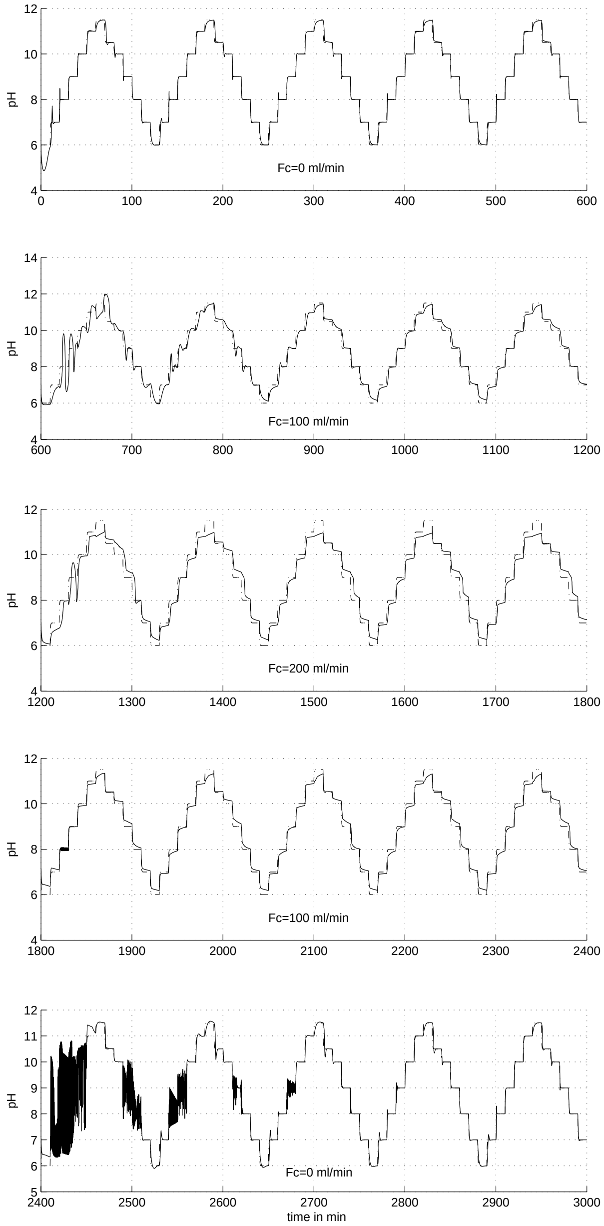

Figure 8: Performance of the adaptive Wiener-model controller when an unknown buffer is introduced

the sampling time are set to be 1 and 1 seconds respectively.

Figure 9 shows the performance of the adaptive neurofuzzy control scheme when the reference pH is varied periodically between 6 and 11.5. By comparing the plots in Figures 5, 7 and 9, it appears that the initial performance of the adaptive neurofuzzy controller pales in comparison the Wiener-model control schemes. A plausible explanation is that a longer time is needed to learn the non-linear pH dynamics, which is more complex. With time, reasonably good tracking control is obtained for pH values between 7 and 9. The ability of the adaptive neurofuzzy controller to reject disturbances in the form of an unknown buffer is shown in Figures 10. Unlike the Wiener-model controllers, the adaptive neurofuzzy controller is able to prevent the carbonic acid from adversely affecting the control performance. This characteristics may be the result of the fact that the adaptive neurofuzzy controller is not constrained by erroneous *a prior* information.

4.4 Discussions

In order to compare the performances of the three controllers objectively, the Integral Absolute Error (IAE) for successive training cycles that comprises of unit step changes from pH = 6 to 12 and back are shown in Figures 11 and 12. The IAE plots indicates that the "black box" approach is better during the first training cycle even though the step responses in Figures 5 and 7 appears to be better than the one in Figure 9. One reason behind the poorer performance of the adaptive Wiener model controller may be that the neurofuzzy controller is used to regulate base ionic concentration when it is trained using a feedback error learning rule that is based on the difference between the desired and actual pH level. When the three controllers have "learnt" the plant dynamics, the "black box" approach still provided the best performance. The same conclusions can also be drawn from the simulations obtained when the characteristics of the pH process were altered by an unknown buffer. Thus, the study seems to suggest that the addition of inaccurate *a priori* information into control structures may hinder the ability of the controller to adapt to process variations. However, generic information, such as the regions where process is sensitive/insensitive to the input, may be used to fine-tune the controller parameters.

5 Conclusions

Control of a pH process using a neurofuzzy controller were studied under nominal conditions and when the pH plant is affected by an unknown buffer. In addition, the pros and cons of utilising structural information to design the controller structure was addressed. The results indicate that the ability of adaptive controllers to adjust to the prevailing conditions may be severely hampered if inaccurate information are incorporated into the controller. Since the exact composition of the reagents in practical pH processes is unknown and disturbances are unavoidable, it appears that the "black box" approach holds the most promise.

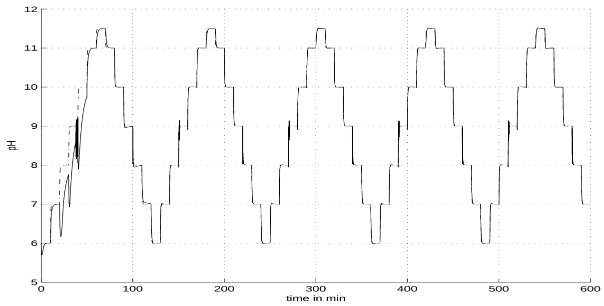

Figure 9: Performance of the adaptive neurofuzzy controller under nominal conditions

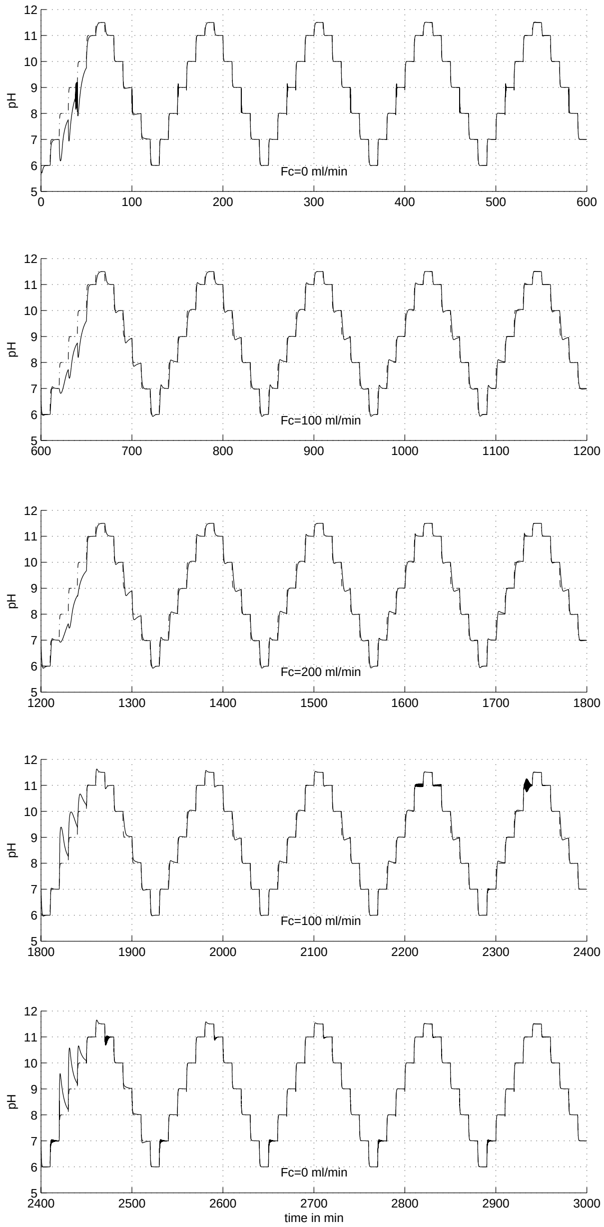

Figure 10: Performance of the adaptive neurofuzzy controller when an unknown buffer is introduced

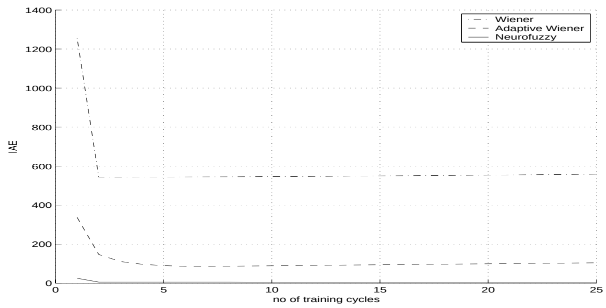

Figure 11: Comparison of IAE between the three controllers under nominal conditions

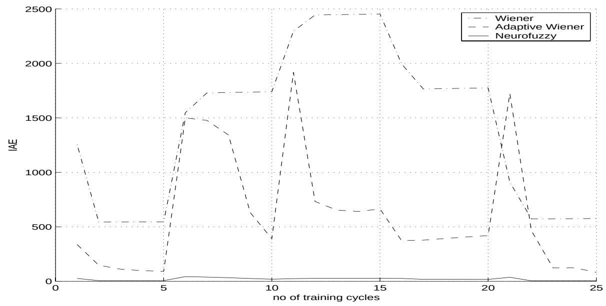

Figure 12: Comparison of IAE between the three controllers in the presence of unknown buffers

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