Vol. 4(1), pp. 1-9, 2025
eISSN: 2976-4009

ASEAN Journal of Process Control

Research Article

Adaptive Neuro-Fuzzy Control of pH and its Derivative in Neutralisation Processes: A Comparative Study

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Abstract: Models for pH and its derivative with respect to base flow rate, dpH/dF_b, were derived for the neutralisation of a strong base-weak acid system. The systems are then controlled and compared through simulation carried out using PI Control, Fuzzy Logic Control (FLC), and Adaptive Neuro-Fuzzy Control (ANFC). Control of dpH/dF_b is an effort made to utilize other phenomenological information of the pH process in a way to improve its control. The dynamics of pH and dpH/dF_b were first compared for various acid/base concentrations and flow rate ratios. The comparison reveals that the dpH/dF_b curve is highly non-linear and more sensitive than the pH neutralisation one. The dpH/dF_b curve is characterized by the singular equivalence point in two sensitivity regions, which makes it a good candidate as a benchmark test to check the effectiveness of non-linear regulatory control strategies for pH. The control of pH and of dpH/dF_b was then compared for the system with and without a time delay. The comparison showed that FLC is superior to the PI controller for the system with time delay for both pH and dpH/dF_b control for various load changes. Because of the multi-sensitivity-region characteristics of the strong base-weak acid system, adaptation of the FLC could enhance the controllability of both pH and dpH/dF_b. An adaptive method for fuzzy logic control of pH and dpH/dF_b was designed, incorporating a neural network in identifying and positioning the membership functions in the FLC and for determining the membership functions' position in the fuzzy logic adapter (FLA) of the scaling factors. The results satisfactorily show that the flexible learning ability of the neural network improves adaptation and the control performance for both pH and dpH/dF_b.

Keywords: neuro-fuzzy control, pH derivative, neutralisation process

1. Introduction

The pH loop has been generally recognized as the most difficult single loop in process control for many reasons. Of these, the response of pH to reagent addition is non-linear, and its sensitivity in the vicinity of the neutral point tends to be extreme, in that a change of one pH unit can result from a fraction of a percent change in reagent addition. In addition, both response and sensitivity are often subject to change in some neutralisation systems. Furthermore, the pH measurement is always associated with a time delay, which aggravates the non-linearity of the system. As a result of these unusual characteristics, many, if not most, pH control loops are unsatisfactory, either limit cycling or slow response to upsets, or both. Considerable efforts and ingenuity have gone into designing advanced control strategies, including non-linear, feedforward, adaptive control, to solve these problems. However, little effort has gone into parametric analysis of the dynamics of the neutralisation process itself to explore other phenomenological behaviour that may lead to developing control systems that are more effective in improving the control of the system. For example, in the case of titrating a weak acid with a strong base, the dynamics of pH amounts to a series of "buffer problems," and the pH curve is characterized by three different sensitivity regions, and its shape is dependent on the process parameters.

Most conventional control techniques for non-linear systems are some forms of linear or non-linear model-based control concepts, which use little phenomenological information of the pH process. Attempts to study the effects of pH process parameters, such as system volume, reagents flow rates, and concentrations on their control have been made. Wilson and Wylupek (1965) and Mellinchamp et al. (1966a) recognized the effect of buffering and attempted to maintain good control by introducing adaptation. Shinskey (1967,1968) proposed feed-forward control by an acid or a base involving valves of different rangeability. Rowton (1968) used a sampled data scheme to control the pH of a large volume neutralisation basin, while the control strategy explored by Hoffmann (1972) involved efficient control in large volume systems through cascade control. Arant (1972) applied ratio control to absorb gross load changes in the flow of the influent to a pH control system, while Jacob et al. (1980) and Proudfoot et al. (1983) used online self-tuning and optimal-k-step-ahead adaptive control to find suitable parameters for the controller. Relative successes in these attempts and others led Gustafsson and Walker (1983) and Jutila and Visala (1984) to study the fundamental properties of a pH process to overcome the difficulties in continuous pH control. They modelled the influent titration curves of monoprotic compounds with user selected aqueous dissociation constant, which was based on prior knowledge of the incoming species. Or modelled the pH process by applying physico-chemical laws that formed the basis for the design of an adaptive control algorithm. MacMillan (1984) stated that the specifications and installation of the components of the experimental set-up formed a potential area for improving pH control, while Shinskey (1973) and More (1978) have presented in detail the technical challenges involved in regulating pH to within narrow limits.

Literature cited above revealed that although the highly non-linear behavior of the pH process can be controlled by conventional methods, an optimum solution is yet to be realized. Detailed investigation of the neutralisation process led to the concept of advanced control to compensate for the non-linearities inherent in the system. Recently, control strategies that include model-based schemes, artificial neural networks, fuzzy logic, adaptive fuzzy logic, and combinations of controls have been employed in pH control systems. Waller and Gustafsson (1983) used the conventional linear model-based PID for pH control, which was found ineffective. Wright et al. (1991) introduced the "strong acid equivalent" to define the control objective, and the results for the strong acid-strong base system showed that the proposed model- based control method can reject disturbances in the presence of model uncertainty. Non-linear model-based controllers have been proposed by Parish and Brosilow (1986), Mahuli et al. (1992), and Costello (1994) with limited success in pH control. The main weakness of many of the proposed non-linear model-based controllers is the lack of robustness caused by the non-linearity of the pH process. To overcome this problem, Gustafsson and Waller (1992) suggested a non-linear and adaptive pH controller, while Mahuli et al. (1993) proposed a "statistical process control cumulative sum" technique for model parameter adjustments. Kulkarni et al. (1991) developed a non-linear internal model control (NIMC) technique, and the model was modified by Shukla et al. (1993) by including a suitable adapter, resulting in what is known as the robust non-linear control law (RNCL) scheme. Wong et al. (1994) applied this model for the control of a strong acid-strong base system at the neutral point in the presence of disturbances, and the results point to the excellent capability of RNCL for controlling pH in comparison to non-linear IMC and PI control. A combination of the concept of adaptation and NIMC present in RNCL for pH control was explored by Narayanam et al. (1997), and the proposed scheme was seen to render robustness to the NIMC as well as tolerance to model uncertainties.

Improved results over those obtained from model-based control of pH are possible if the inherent problem of modeling the system is overcome by making the model equation mimic a real-time process. The use of neural networks in pH control reduced the difficulties associated with the model-based approach. Tambe et al. (1996) discussed in detail the use of neural network-based control of pH. Aoyama et al. (1996) proposed the concept of using a fuzzy-neural network in an IMC strategy for pH control. The network was trained using steady-state and transient data by back propagation. However, the main drawbacks of the neural network method lie in the fact that the generalized delta rule is computationally complex when the training data are numerous, and the learning time can be very long.

Fuzzy logic-based control has been recommended for complex, ill-defined, non-linear processes where human experience has an edge over the mathematical models (Rhinehart et al., 1996). FLC provides a flexible means of implementing intelligent non-linear control and has been widely used in the control of pH (Jager et al, 1994; Parekh et al., 1994; Qin and Borders, 1994; Heckenthaler and Engell, 1995; and others). FLC utilizes scaling factors to scale error, change in error, and membership functions to direct the decision process. Combinations of this 'model-free' FC with other learning algorithms, such as neural networks, genetic algorithms, to adapt the fuzzy parameters has been the focus of recent research on pH control (Galluzzo et al.,1991; Karr and Gentry, 1993). From this brief survey on pH control, it can be seen that improved results may be obtained if the model equations were to mimic a real-time process subjected to various operating conditions in order to gain enough insight into the phenomenological behavior of the pH process. On the control side, it seems that adopting strategies based on adaptive fuzzy control may lead to better control of the neutralisation process.

The first objective of this study is to develop model equations for the pH and for dpH/dF_b systems of weak acid-strong base neutralisation, followed by parametric analysis of their dynamics, and comparison of the simulated titration curves with what is available in the literature. Second objective: to compare, by simulation, the controllability of FLC and PI controllers for both pH and dpH/dF_b systems with and without time delay. The final objective is to design an adaptive neuro-fuzzy controller for scaling factors adaptation to enhance the controllability of pH and dpH/dF_b at the neutral point and to enable effective pH control outside the neutralisation region.

2. Materials and Methods

2.1 pH Model

Consider an isothermal, perfectly mixed, continuous stirred tank of constant volume,V, into which sodium hydroxide solution of concentration Cb flows in at rate Fb to neutralize an acetic acid stream of concentration Ca flowing at a rate Fa. The manipulated variable is Fa, and the system is controlled with respect to set point pH_s or $(dpH/dFb)_{max.}$ with Fb, Ca, and Cb as load disturbances. Unsteady state component material balances of acetic acid and sodium hydroxide yield:

$$V\frac{dxa}{dt} = Fa \times Ca - (Fa + Fb)xa \tag{1}$$

$$V\frac{dxb}{dt} = Fb \times Cb - (Fa + Fb)xb \tag{2}$$

Where, $xa = [CH3COO^-] + [CH3COOH]$, $xb = [Na^+]$

The electroneutrality balance yields:

$$[H^+] + [Na^+] = [CH3COO^-] + [OH^-] \tag{3}$$

Substituting for the dissociation constant of acid, Ka, and that of water, Kw, into Eq.(3) and simplifying yields:

$$[H^+]^3 + (Ka + xb)[H^+]^2 + ((xb - xa)Ka - Kw)[H^+] - Ka \times Kw = 0 \tag{4}$$

If the concentration of acetic acid is chosen such that the ratio Ka/Cb < 0.001, then ionic concentrations can be used instead of activities (Wallace,1958). Solving Eqs.(1)-(4) simultaneously, and using the relationship: $pH = -\log_{10}[H^+]$, would give the dynamic behavior of the system's pH.

2.2 dpH/dFb Model

Integrating Eq.(1) and Eq.(2) between two conditions, then differentiating with respect to Fb yields:

$$\frac{dxa_2}{dFb} = Fa \times Ca\left[\frac{(Fa+Fb)(\Delta t/V)e^{-\frac{(Fa+Fb)\Delta t}{V}} - (1-e^{-\frac{(Fa+Fb)\Delta t}{V}})Cb}{(Fa+Fb)^2}\right]$$

$$-xa_1(\Delta t/V)e^{-\frac{(Fa+Fb)\Delta t}{V}} + \frac{dxa_1}{dFb}e^{-\frac{(Fa+Fb)\Delta t}{V}} \quad (5)$$

$$\frac{dxb_2}{dFb} = \left[\frac{(Fa+Fb)[Fb \times Cb(\Delta t/V)e^{-\frac{(Fa+Fb)\Delta t}{V}} + (1-e^{-\frac{(Fa+Fb)\Delta t}{V}})Cb(1+Fb)}{(Fa+Fb)^2}\right]$$

$$-xb_1(\Delta t/V)e^{-\frac{(Fa+Fb)\Delta t}{V}} + \frac{dxb_1}{dFb}e^{-\frac{(Fa+Fb)\Delta t}{V}} \quad (6)$$

Differentiating the relation: pH = $-\log_{10}[H^+]$ w.r.t. Fb yields:

$$\frac{dpH}{dFb} = -\frac{1}{\ln 10}\frac{1}{[H^+]}\frac{d[H^+]}{dFb} \quad (7)$$

Differentiating Eq.(4) w.r.t. Fb and substituting Eq.(7) yields:

$$\frac{dpH}{dFb} = \frac{[H+]\times\frac{dxb}{dFb} + Ka(\frac{dxb}{dFb} - \frac{dxa}{dFb})}{3[H+]^2 + 2[H+](Ka+xb) + (xb-xa)Ka - Kw}\frac{1}{\ln 10} \quad (8)$$

Solving Eq. (4) first and then substituting the value of $[H^+]$ together with other parameters, Eq. (8) can be solved.

2.3 Fuzzy Logic Controller

Conceptually, the system architecture for the fuzzy control scheme is shown in the figure. 2. The measured pH, pH_m, is fed back to the controller and is compared with the desired pH, pH_{sp}. The input to the controller is e_t, which is the difference between pH_{sp} and pH_m at any given time, and any given time, and Δe_t, which is the change in e_t at the sampling time. The output Δu_t is added to the previous u_{t-1} to produce the manipulated variable u_t, such that the pH of the overall system follows the set point asclosely as possible.

A typical fuzzy logic controller (FLC) is composed of three basic parts: input signal fuzzification, a fuzzy engine that handles rule inference, and a defuzzification part that generates continuous signals for an actuator such as a control valve (Figure 3). The fuzzification block transforms the continuous input signals into linguistic fuzzy variables such as Small, Medium, and Large. The fuzzy engine carries out rule inference where human experience can easily be injected through linguistic rules. The defuzzification block converts the inferred control action back to a continuous signal that interpolates between simultaneously fired rules [3].

Two distinct features of fuzzy logic control are that:

- human experience can easily be integrated, and
- fuzzy logic provides a non-linear relationship induced by membership functions, rules, and defuzzification.

These features make fuzzy logic promising for process control, where conventional control technologies can only provide moderate performance. Furthermore, the presence of human knowledge and experience makes fuzzy logic control even more credible. The enhanced performance of fuzzy control can be demonstrated in both the transient and steady responses. If the system tends to have changed dynamic characteristics or exhibits non-linearities, fuzzy logic control should offer better alternative than constant PID settings.

2.4 Adapt Neuro- FLC

From previous studies, the performance of FLC deteriorates when the control action moves towards a region outside the neutralisation region. This happened due to the highly non-linear nature of the neutralisation system and the changes in the dynamics of the neutralisation process with time. Among the various adaptive techniques being reviewed, adaptation of FLC using a neuro-fuzzy as an adapter had been chosen for pH control of this neutralisation process due to its learning ability. In the previously designed adaptive FLC [4], two scaling factors are adapted at one time to improve the control performance. However, if the correct choice of membership functions were employed using neuro-fuzzy, a one-scaling factor adaptation would be sufficient to ensure good cross-regional set points tracking.

Prior to deciding on which parameter is to be adapted, the effect of each scaling factor on the system behaviour has to be observed, for changes in set points, e.g., from pH 7 to pH 8. As from the trial run, the effects of k_e and k_{du} on the response of the system are more or less the same. Increasing the value of k_e and k_{du} gives a faster response and hence shorter settling time. However, if these values are too high, oscillation will occur. On the other hand, the value of k_{de} does not affect the rise time and settling time of the response. However, the system becomes unstable if a value of k_{de} that is too high is used. With the above information, it is decided to adapt k_{du}. This is because the magnitude of k_{du} governs the manipulated variable, base flow rate, F_b, which has a more direct effect on the overall performance of the controller.

Here is an example of how the neuro-fuzzy adapter for k_{du} is developed. The current error, $e_{n,}$ and the current pH set point, pH_{sp}, had been chosen to be the input variables of the k_{du} adapter as shown in Figure 4. These two variables could well define the process condition. As opposed to FLC, the linguistic rules for the training data are presented in the form of numerical values rather than attributes. The procedure of obtaining training data for network learning is established as follows. The non-adaptive FLC was simulated so as to obtain the respective k_{du} that gives good control from several changes in different regions. The optimum values of k_{du} are shown as in Table 1. The table represents the numerical form of linguistic rules, which are in the form of an if-then format. For example, if pH_{sp} is 5 and e_n is –8, then k_{du} is 0.3. Various simulations were performed using this adaptive neuro-fuzzy control strategy. The simulations were done for set points tracking from various pH. These were also done for cases without system delays and with delays. They are compared to that of FLC without adaptation. Figure 5 shows that the adaptive neuro-fuzzy logic controller tracks the set point better.

3. Results and Discussion

3.1 *Analysis of Neutralisation Curves*

Based on the model equations developed, programs were written for the generation of the dynamic and steady state behavior of the two systems. Steady state neutralisation curve and its derivative w.r.t Fb, using the nominal values of: V = 10 L; Fa = 2 L/min; Ca = Cb = 0.05 M; Ka = 1.75*10^(-5); Kw = 10^(-14), as shown in Figure 1 and Figure 2. As can be seen from Figure 1., the neutralisation curve is characterized by three sensitivity regions: the acidic region (I) where the pH changes gradually with Fb and its sensitivity may be classified as moderate; the neutralisation region (II) where the pH changes sharply with Fb and its sensitivity is high; the basic region (III) where complete dissociation of the strong base causes sensitivity to be low. In Figure 2. the dpH/dFb curve is a spike resembling an impulse. As a result, it is characterized by two sensitivity regions: regions (I&III) are low sensitivity regions, while the neutralisation region (II) is highly sensitive compared to the pH high sensitivity region. In the pH system, a change of 0.2 L/min of reagents around the neutralisation region may affect the pH along the span of 6-11, while a similar change in the dpH/dFb system may cause the values of dpH/dFb to react between the span of 10-700 or even higher. Figure 3 shows the behavior of the dpH/dFb versus Fb system with respect to changes in the ratio Ca/Cb. The maximum point $(dpH/dFb)_{max}$ corresponds to the equivalence point of the neutralisation system, a state when equal amounts of acid and base are added together. This shows that at this point the pH is not always 7 and shifts away from 7 with change in reagent concentration ratio. It should be noted here that the locus of maxima is an exponential decay, and similar behavior was observed when changing Fa while maintaining the ratio Ca/Cb = 1. Figure 4 shows the behavior of the dpH/dFb versus Fb for various Fa values keeping the ratio Ca/Cb = 1 but varying the reagent concentrations from their nominal value of 0.05M. Again, a visible difference in the maxima of the dpH/dFb system is observed, and Figure 5 shows the equivalent pH curve as a function of Ca., and it can be concluded that the equivalence point continues to deviate according to change in Ca or Cb even if the value of Ca/Cb is kept constant at 1. This parametric analysis of the behavior of dpH/dFb versus Fb shows that the use of this system in pH control is only limited to regulatory control and that changes in Fa, Ca and Cb should be limited so that the equivalence point shift becomes insignificant.

3.2 Comparisons of System-Controller Combinations

The comparisons are made between PI control of pH and dpH/dFb, FLC of pH and dpH/dFb and ANFC of pH and dpH/dFb in order to demonstrate the robustness of the pH control system to be chosen. As shown earlier, the dpH/dFb /Fb system is non-linear, highly sensitive and experiences shift in equivalence pH when conditioning parameters such as Fa, Ca, and Cb are changed. Therefore, it is used here as a benchmark test to check the effectiveness of the control strategy. In the comparisons, the change in loads is limited to within ± 10% of the nominal values when controlling dpH/dFb and that ensures less than 0.1% change in equivalent pH.The effectiveness of any one controller-system is based on pH- dpH/Fb plots and the numerical values of the rise time, settling time, ITAE, percent overshoot, decay ratio and offset. Ziegler-Nichols method was used for tuning the PI controller for pH and by trial-and-error for PI- dpH/Fb. A trial-and-error procedure was also followed for tuning the FLC scaling factor for both systems, though it was tedious for dpH/Fb due to the absence of prior information for the initial guess. The results of these tunings are shown in Table 1.

Table 1. Tunings for System-Controller Combinations

Control System	Controller	Tunings
pH	PI	P = 0.0025 I = 0.0010
	FLC	Ke = 0.080 Kde = 1.15 Kdu = 0.005
dpH/Fb	PI	P = 0.00001 I = 0.000002
	FLC	Ke = 0.0010 Kde = 0.0140 Kdu = 0.0004

At this stage, the combinations of systems and controllers are subjected to load changes in Fa, Ca and Cb without and with time delay of 1 minute. As an example, the results for the case of step change in Cb with time delay are shown in Figure 6 and Table 2.

Table 2. Performance Analysis for Cb Load Change with Time Delay

System	Controller	Rise Time (min)	Settling Time (min)	ITAE (min)	% Overshoot	Decay Ratio	Offset
dpH/dFb	PI	Osc	Osc	410.5	Osc	Osc	Osc
dpH/dFb	FLC	44	74	90.45	31.9	0.24	0
pH	PI	90	93	182.5	32.2	0	0
pH	FLC	24	53	52.09	31.0	0.24	0

The results for the step change in other loads showed similar performance behavior. It can be seen from these results that the more robust FLC can perform way above that of a conventional PI controller, especially under the demanding conditions of the dpH/dFb where the response was oscillatory under PI control. The obvious performance of FLC is the improvement in the rise and settling times. Due to the multi-region dynamics of the pH and dpH/dFb systems, the controller settings may not perform as expected when the system is subjected to load changes or when the set point is moved away from the neutralisation region. Therefore, the second stage is to test the performance of the FLC under adaptation. In a previous study (Elkanzi and Hussain,2000) a fuzzy logic adapter was used to adapt the scaling factors Ke and Kde of the FLC at one time to improve the performance. However, if the correct choice of membership functions were employed using neuro-fuzzy, a one scaling factor adaptation would be sufficient to ensure good cross-regional set point tracking. The adapter used here is the neuro-fuzzy adapter (NFA) with two inferring variables, pHs and error, for the pH system and $(dpH/dFb)_{max}$ for dpH/dFb system to adapt Kdu. As an example, the results for a step change in Cb coupled with a time delay are shown in Figure 7 and Table 3.

Table 3. Performance Analysis for Cb Load Change with Time Delay

System	Controller	Rise Time (min)	Settling Time (min)	ITAE (min)	% Overshoot	Decay Ratio	Offset
dpH/dFb	ANFC	33	62	74.07	31.6	0.53	0
pH	ANFC	17.7	40	39.98	29.4	0.603	0

From these results, it is clear that the ANFC outperforms the FLC with improvements of 26.25% and 24.5% in rise and settling times for pH control and of 25% and 16% for the highly sensitive dpH/dFb control. Finally, Figure 8 compares set point tracking of the ANFC and FLC due to a step change in set point without a time delay. The ANFC was able to track set point change ahead of FLC, where settling time is greatly improved, though overshoots are rather obvious.

4. Conclusions

Parametric analysis of the dynamics of the neutralisation of acetic acid and sodium hydroxide revealed that the dynamics of the derivative of pH w.r.t. flow rate, dpH/dFb, yield a highly non-linear and sensitive model in the vicinity of the equivalence point compared to the dynamics of pH itself. Thus, the model is used as a benchmark test to check the effectiveness of non-linear regulatory control strategies of pH. From the simulation results of comparative analysis of system-controller combinations, the following may be concluded:

- When subjected to dpH/dFb control, the conventional PI controller is a poor candidate for the pH control of the neutralisation of acetic acid and sodium hydroxide, and the response becomes oscillatory in the presence of time delay.

- The fuzzy logic controller outperforms the PI controller in pH control and passed the dpH/dFb test under a variety of load changes with and without time delays.
- A neural network is used to adapt one scaling factor, Kdu, in a fuzzy logic adapter and to properly assign membership functions within the FLC itself. This adaptive-neuro-fuzzy controller was subjected to dpH/dFb controluo and the results have demonstrated the capability of using neuro–fuzzy both as an adapter and controller for pH control. The results were demonstrated for load rejection with and without time delays and for set point tracking. The ANFC outperformed the non-adaptive FLC in all situations studied.

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