1982

Adaptive Feedforward Control of Wastewater Neutralization.

Richard Albert Balhoff

Louisiana State University and Agricultural & Mechanical College

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ADAPTIVE FEEDFORWARD CONTROL
OF WASTEWATER NEUTRALIZATION

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by

Richard Albert Balhoff
B.S.Ch.E., Louisiana State University, 1977
M.S.Ch.E., Louisiana State University, 1979
August 1982
DEDICATION

This dissertation is dedicated to my parents, without whose endless love and assistance this accomplishment would have been impossible.
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ABSTRACT

The purpose of this dissertation is to show the development and testing of an adaptive feedforward control of a wastewater neutralization process. The adaptive controller is compared to a nonlinear proportional-integral-derivative (NPID) controller developed by Shinskey (1970). The process and controllers were simulated digitally. The adaptive controller utilizes two pH probes, a feedforward probe and a feedback probe (this measurement is used in the adaptive gain calculation). The feedback measurement provides the adaptive controller with a form of reset action. Probe noise and lag, valve hysteresis and lag, and dead time were included in the simulation.

The process simulated for control combines a strong (hydrochloric) and weak (carbonic) acid neutralized by a strong base (sodium hydroxide). The adaptive controller was shown to give superior responses both for step changes in the strong acid and the buffer (weak acid) concentration.

The tuning constant limits for the adaptive controller are correlated versus the buffer concentration of the incoming solution for a base case. The sensitivity of the adaptive control to changes in certain parameters (probe noise and lag, valve hysteresis and lag, and dead time) are illustrated. Also shown is the effect of a step change in
flow rate to the system. Noise in the feedforward pH probe and the dead time between the reagent addition and the feedback probe had the largest effect on the adaptive controller performance.

Efforts to solve the many problems involved in the control of the pH of effluent streams have failed to yield acceptable control algorithm for this very difficult process. This research provides a significant step toward the solution of these problems. An additional bonus of the adaptive controller is the use of only two tuning parameters (many controllers in use today require five or more tuning parameters).
CHAPTER I
INTRODUCTION

Waste neutralization has long been an extremely difficult process to control. This is due mainly to the wide variations in gain across the range in pH and also large gain changes due to changes in the relative amounts of strong and weak acids and bases with time. These fluctuations can effect gain changes of several decades. Obviously, these characteristics place severe demands on the typical linear controller.

Most of the industry has attacked the pH problem by using large settling ponds with reagent addition between each pond to bring the pH within the acceptable range. As restrictions on the effluent pH continue to tighten and costs escalate, the necessity for a more efficient control scheme becomes more apparent.

In 1970, Shinskey applied a more sophisticated control than the standard linear PID controller to an industrial wastewater treatment. The scheme employed three controllers: a feedforward, an adaptive nonlinear feedback, and a proportional feedback controller. Several parameters had to be adjusted, most of them manually, to accomodate the changes in the process parameters. In 1973, he further modified this technique by eliminating the trim controller.
and adding some additional parameters to the remaining scheme (crossover frequency, low-frequency gain and adaptive reset) to try to handle the nonlinearities and rapid changes in process conditions. In 1979, Shinskey simplified his design in his control book, but he gave no indication of its control performance.

Niemi, et al. (1977) attempted to solve the nonlinearity problem by using a variable transformation to introduce a new variable, \( C \) (where \( C = [H^+] - [OH^-] \)), to be controlled instead of the actual pH. The strong acid-strong base system which they tested reacted slightly better to this variable. However, as they pointed out, the addition of weak acids and bases disrupts the linear characteristic of the variable and can create gain changes of several decades. This is a severe problem when dealing with real systems which always contain varying amounts of buffering agents.

Gupta, et al. (1978) investigated an adaptive feedback control scheme in which the process gain was estimated by pulsing reagent to a small identification tank. This gave stable control and eliminated the limit cycling which developed in the non-adaptive controller but required an additional tank and the diversion of part of the flow through this tank.

Bucholt, et al. (1979) used the linear variable transformation and a recursive algorithm to adapt feedback parameters. Stable control was achieved but long periods
(approximately one hour) were required for the parameters to reach their new values, thereby reducing the oscillations in pH. They also dealt only with strong acids and bases.

Davaloo, et al. (1979) studied the control of pH with conventional PID controllers. They achieved reasonable control with two tanks but only with the simplified system of strong acids and bases.

Ricter, et al. (1979) studied the use of a sustained limit cycle in a bypass pipe to estimate the process gain. The method, however, only estimated the gain immediately around neutral so that upsets which drove the pH out of this range were still troublesome. Also, no dynamic testing of the control scheme was done to indicate the effectiveness of the control algorithm for gain changes.

Trevathan (1978 and 1979) reviewed the literature on pH control. He provided general guidelines for improving the controllability of a pH process but referred to pH control as "one of the most difficult single dimension control problems in the process industries despite considerable research and publication efforts..." (1978).

Gray (1980) described a microprocessor-based controller which utilized a characterized pH. The algorithm required the adjustment of the three PID parameters plus five additional parameters to custom fit the characterized pH function to a neutralization curve. Since each of these eight constants must be set manually (and a neutralization curve must be obtained to set the five customizing
parameters), it would be difficult to maintain proper tuning for rapidly changing process parameters. In addition, many systems could not be represented properly by the S-shaped curve used for the pH characterization.

Control of pH continues to be a formidable problem. The studies which have been done have either used too simple a system or have developed schemes which require manual adjustment of several control parameters as process parameters change. These systems are not very efficient in the complex and rapidly changing process conditions usually present in wastewater neutralization process.

In an attempt to solve some of the shortcomings of these previous control schemes, an adaptive feedforward controller has been developed using a digital simulation of a wastewater neutralization process. Chapter 2 shows the mathematical development of the process and the controller simulation. Chapter 2 also presents the equations for a nonlinear proportional-integral-derivative (NPID) controller proposed by Shinskey (1970). This controller has been implemented on many industrial processes and is used to gauge the effectiveness and stability of the proposed controller.

The adaptive controller performance is compared to that of the NPID controller for various levels of the strong and weak acid concentrations in Chapter 3. The effect of these acid levels on the tuning of the adaptive controller are studied in this chapter.
Chapter 4 discusses the sensitivity of the adaptive controller to various parameters (probe noise and lag, valve hysteresis and lag, dead time, tank capacity, and feedforward intercept). Controller response to flow rate changes are also addressed.
CHAPTER II
DEVELOPMENT OF PROCESS AND CONTROLLER MODELS

Introduction

This chapter will: 1) develop the mathematical models needed for the simulation of the pH process (mixed tanks, pH probes, valves, and dead times), 2) give a brief explanation of a nonlinear PID controller developed by Shinskey (1973) which will be used as a standard for comparison of the proposed controller, 3) show the development of the proposed controller and the equations which define it.

Process Models

The modeling equations will be developed for the mixed tank shown in Figure 2-1. The results can easily be modified for any number of inputs.

The system under study consists of water, sodium hydroxide (NaOH), hydrochloric acid (HCl), and carbonic acid (H₂CO₃). The ionization reactions are:

\[ \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{OH}^- \quad (1a) \]
\[ \text{H}_2\text{CO}_3 \rightarrow \text{H}^+ + \text{HCO}_3^- \quad (1b) \]
\[ \text{HCO}_3^- \rightarrow \text{H}^+ + \text{CO}_3^{2-} \quad (1c) \]
Figure 2-1
Mixing tank with two inputs and one output
The sodium hydroxide and hydrochloric acid completely ionize.

**Material Balances:** Balances must then be performed on the species which are not consumed or generated. The following species are conserved:

\[
x = [\text{Cl}^-] \quad (2a)
\]
\[
y = [\text{Na}^+] \quad (2b)
\]
\[
z = [\text{H}_2\text{CO}_3] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}] \quad (2c)
\]

Then writing the material balances in the form

\[
\text{Accumulation} = \text{In} - \text{Out} \quad (3)
\]

yields

**Cl balance:**
\[
\frac{d(V \cdot x)}{dt} = (F_1 \cdot x_1 + F_2 \cdot x_2) - F_0 \cdot x_0 \quad (4a)
\]

**Na balance:**
\[
\frac{d(V \cdot y)}{dt} = (F_1 \cdot y_1 + F_2 \cdot y_2) - F_0 \cdot y_0 \quad (4b)
\]

**Carbonate balance:**
\[
\frac{d(V \cdot z)}{dt} = (F_1 \cdot z_1 + F_2 \cdot z_2) - F_0 \cdot z_0 \quad (4c)
\]

**Volume change:**
\[
\frac{dV_0}{dt} = (F_1 + F_2) - F_0 \quad (4d)
\]
If the volume of the tank is assumed to be constant, then

\[ F_o = F_i + F_z \]  

(5)

and

\[
\frac{dx_o}{dt} = \frac{(F_i \cdot x_i + F_z \cdot x_z) - (F_o/V_o) \cdot x_o}{V_o}, \quad (6a)
\]

\[
\frac{dy_o}{dt} = \frac{(F_i \cdot y_i + F_z \cdot y_z) - (F_o/V_o) \cdot y_o}{V_o}, \quad (6b)
\]

\[
\frac{dz_o}{dt} = \frac{(F_i \cdot z_i + F_z \cdot z_z) - (F_o/V_o) \cdot z_o}{V_o}, \quad (6c)
\]

Since these equations are independent, they can be solved separately, yielding

\[
x_o = x_o(0) \cdot \exp(-\frac{F_o}{V_o} \cdot t) + \frac{1 - \exp(-\frac{F_o}{V_o} \cdot t) \cdot (F_i \cdot x_i + F_z \cdot x_z)}{F_o}, \quad (7a)
\]

\[
y_o = y_o(0) \cdot \exp(-\frac{F_o}{V_o} \cdot t) + \frac{1 - \exp(-\frac{F_o}{V_o} \cdot t) \cdot (F_i \cdot y_i + F_z \cdot y_z)}{F_o}, \quad (7b)
\]

\[
z_o = z_o(0) \cdot \exp(-\frac{F_o}{V_o} \cdot t) + \frac{1 - \exp(-\frac{F_o}{V_o} \cdot t) \cdot (F_i \cdot z_i + F_z \cdot z_z)}{F_o}, \quad (7c)
\]

if \( F_i, F_z \), and the inlet concentrations are constant over \( t \) (this is a good approximation for a small time step, \( \Delta t \)). The variables \( x_0(0), y_0(0), \) and \( z_0(0) \) are the tank concentrations at time \( = 0 \). The quantities \( V_o/F_o \) and
\[(F_1 \cdot x_1 + F_2 \cdot x_2)/F_0 \text{ are the time constant of the system and the average inlet concentration of } x, \text{ respectively. These approximations are used at each time step, } \Delta t \text{ to obtain the concentrations } x_0, y_0, z_0 \text{ by the recursive formulae}
\]

\[x_0(n) = x_0(n-1) \cdot a + \frac{(F_1 \cdot x_1 + F_2 \cdot x_2)(1 - a)}{F_0}, \quad (8a)\]
\[y_0(n) = y_0(n-1) \cdot a + \frac{(F_1 \cdot y_1 + F_2 \cdot y_2)(1 - a)}{F_0}, \quad (8b)\]
\[z_0(n) = z_0(n-1) \cdot a + \frac{(F_1 \cdot z_1 + F_2 \cdot z_2)(1 - a)}{F_0}, \quad (8c)\]

where \( a = \exp(-F_0/V_0) \cdot \Delta t \).

**Equilibrium Equations:** The dissociation equilibrium equations must also be satisfied for this system. These are as follows:

**Carbonate equilibrium:**

\[\frac{[H^+][HCO_3^-]}{[H_2CO_3]} = K_{b1} = 4.46 \times 10^{-7} \quad (9a)\]

\[\frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} = K_{b2} = 5.61 \times 10^{-11} \quad (9b)\]

**Water equilibrium:**

\[[H^+][OH^-] = K_w = 1 \times 10^{-14} \quad (9c)\]

**Electroneutrality:** Since the solution must be electrically neutral, the following condition must also hold:
\[ [H^+] + y = [OH^-] + [HCO_3^-] + 2[CO_3^{2-}] + x \]  \hspace{1cm} (10)

**Calculation of pH**: Combining the equilibrium equations with the condition of electroneutrality and the definition of "z", yields

\[
[H^+]^a + (K_{b1} + y - x) \cdot [H^+] \cdot 
(K_{b1} \cdot (y - x - z) + K_{b1} \cdot K_{b2} - K_w) \cdot [H^+] \cdot 
(K_{b1} \cdot K_{b2} \cdot (y - x - 2z) - K_w \cdot K_{b1}) \cdot [H^+] -
K_w \cdot K_{b1} \cdot K_{b2} = 0
\]  \hspace{1cm} (11)

This equation can be solved for \([H^+]\). The pH of the solution can then be calculated by the definition of pH:

\[ \text{pH} = -\log_{10}[H^+]. \]  \hspace{1cm} (12)

The most stable solution of eq.(11) is interval halving of the pH over the interval 0 to 14. These pH values are then transformed into hydrogen ion concentrations (trial and error guesses) for substitution into eq.(11) by

\[ [H^+] = 10^{-\text{pH}}. \]  \hspace{1cm} (13)

Selected neutralization curves for this system (calculated from eq.(11)) are shown in Figure 2-2. These curves are identical to the neutralization curves reported for zero and 0.005 mol/l carbonic acid by Shinskey (1973).
Figure 2-2
Neutralization curves
(reagent added is relative to amount required to neutralize to 7)
**pH Probe Dynamics:** It has been reported that the dynamics of a pH probe can be approximated by a first order lag. However, studies have shown the time constant of the lag is dependent on whether the pH is moving toward or away from neutral (McAvoy, 1979). The time constant moving away from neutral is approximately double that in the reverse direction. Since this should have only a small effect on the control response, the time constant has been assumed to be the same in both directions as suggested by Marra (1979). The validity of this assumption will be discussed in Chapter 4.

The probe lag can be simulated by a digital filter similar to the one obtained in the solution for the mixing tank concentrations,

\[ pH(n) = pH(n-1) \cdot a_p + pH_s \cdot (1 - a_p), \]  \hspace{1cm} (14)

where \( a_p = \exp(-\Delta t/\tau_p) \).

"n" is the step number, \( \Delta t \) is the time step for the simulation and \( \tau_p \) is the time constant of the probe. For the base cases presented in Chapter 3, this time constant will be set at one second.

**pH Probe Noise:** Fluctuations in concentrations around the pH probe and electrical noise cause the measurement of the pH to be distributed around a mean value. This noise was simulated by adding a uniformly distributed random variable with a maximum absolute value and a mean of zero to
the calculated pH value to give the pH transmitted to the controller:

\[ \text{pH}_t(n) = \text{pH}(n) + w(n), \] (15)

where \( w(n) \) is the randomly distributed measurement error with a maximum absolute value, \( w_{\text{max}} \). The base cases discussed in Chapter 3 will be made with this value equal to 0.01 pH units for the probes immediately after a mixed tank. Since more noise would be expected from the incomplete mixing at the feedback probe for the adaptive control scheme, a value of 0.1 pH units will be used for this probe in the base cases.

**Valve Dynamics:** It would be nice if valves opened instantaneously to the proper position. In reality, however, valves require a finite time to move to a new position. Also, the valve will never actually reach the desired position and upon reversal of direction will actually remain stationary until a given change in air pressure occurs. The lag is a result of the mass of the valve. The inaccuracy of the valve position is caused by friction on the valve stem and is commonly referred to as "hysteresis" or "valve sticking".

Valve hysteresis is caused by friction in the control valve stem. This friction acts in the opposite direction of the driving force created by the difference between the air to the valve and the valve spring but cannot be greater than
this force. This is shown mathematically as

\[ F_t = \text{sign}(F_a - F_s) \cdot \min(F, \max|F_a - F_s|) \]  \hspace{1cm} (16)

where
- \( F_t \) = force of friction on the valve stem,
- \( F_a \) = force applied by the air on the control valve,
- \( F_s \) = force applied by the valve spring.

The driving force for valve movement in terms of fraction of valve movement is obtained from the spring constant and the maximum distance of valve movement and is given by

\[ m_a - m_s + m_f = \text{driving force for movement}, \] \hspace{1cm} (17)

where
- \( m_a \) = signal from controller,
- \( m_s \) = valve position,
- \( m_f \) = stem friction as a fraction of full movement.

Since the valve is approximately a first-order lag,

\[ \frac{dm_a}{dt} = (m_a - m_s + m_f), \] \hspace{1cm} (18)

where \( \tau_v \) = time constant of the valve.

A valve positioner (a proportional controller acting on the error in the valve position) is a necessity to achieve the accuracy of reagent addition required. If a valve positioner is added to the dynamic equation above, it
becomes

\[
\frac{dm_a}{dt} = \frac{1}{\tau_v} \left( K_{vp} \cdot (m_a - m_s) - m_s + m_f \right). \tag{19}
\]

Rearrangement yields

\[
\frac{dm_a}{dt} = \frac{K_{vp}}{\tau_v} \left( m_a - \frac{(K_{vp} + 1)\cdot m_s + m_f}{K_{vp}} \right). \tag{20}
\]

It can be seen then that a valve positioner with a large gain, \( K_{vp} \), decreases both the effective time constant, \( (\tau_v/K_{vp}) \), and the effective hysteresis, \( (m_s/K_{vp}) \), of the valve. The valve simulation will use these effective values. These effective values will be one second and 0.5\% of the total valve movement, respectively, in the base cases in Chapter 3.

**Valve Sequencing:** Since the amount of electrolytes present in a waste stream can vary over a very wide range, the control valve must also be able to accurately deliver reagent over a wide range. Shinskey (1973) shows that the best way to achieve the necessary rangeability is by sequencing (or coupling) two (or more) equal-percentage valves. Two equal-percentage valves having rangeabilities of 50:1 could be sequenced to achieve an equivalent equal-percentage valve of up to 2500:1. In practice, a reasonable overlap of the valves is desirable, yielding something closer to 1000:1. Figure 2-3 shows an example of
Figure 2-3
Sequencing of two equal-percentage valves
(Shinskey, 1973)
this sequencing on a semi-log plot. This arrangement would require the larger valve to be twenty times the size of the smaller valve. Note that only one valve should be open at any given time. The valve positioners must be properly adjusted to achieve this coupling. A pressure switch (which includes hysteresis) can be used with solenoid valves to select the proper valve depending on controller output. For example, the large valve should open when the control signal rises to 57% (maximum flow for the small valve), while the small valve closes, whereas when the control signal drops to 43% (minimum flow for the large valve), the large valve should close as the small valve opens. This procedure eliminates the switching back and forth between the valves when around the switch point. A simple schematic of the valves is presented in Figure 2-4.

The valve combination is, therefore, modeled as one valve with the range of 1000:1. It is expressed mathematically as

\[
F_v = F_{v_{\text{max}}} \cdot R \cdot (1 - m)
\]

(21)

where

- \( F_v \) = flow rate through valve
- \( F_{v_{\text{max}}} \) = maximum valve flow rate through valve
- \( R \) = range of valve (i.e., 1000)
- \( m \) = signal to valve (0 to 1)

**Dead Times**: The mixing tanks in this simulation will be approximated by a lag-plus-deadtime model. The lag is the
Figure 2-4
Schematic of valve sequencing
dominant time constant of the tank and the dead time is an approximation of the apparent dead time caused by incomplete mixing, smaller time constants, and pipe flow before the pH measurement. This effective dead time will be assumed to be one second for the base cases discussed in Chapter 3.

These (and any other dead times in the simulation) will be approximated by storing the concentrations \( x, y, \) and \( z \) for \( N_d \) time steps (\( N_d = \) dead time/time step size). These concentrations can then be used to calculate the hydrogen ion concentrations and therefore the pH of the solution at that point in time.

**Shinskey's Nonlinear PID Controller**

It is desirable, when developing a new method, to have a standard for comparison. This helps to identify the relative strong and weak points of the proposed method. Ideally, the standard should be fairly advanced yet well established and used in numerous industrial applications.

The control method chosen as a standard in this work was developed by Shinskey (1970) and meets the qualifications listed above. The method is a nonlinear proportional-integral-derivative controller utilizing a characterized pH. Shinskey reported the industrial application of this controller in this same paper (1970). This controller will be briefly discussed below. For a more detailed treatment of this controller, consult Shinskey's book on pH and pIon control (1973).
**Characterized pH:** Since the neutralization curve for most systems is highly nonlinear, control with a linear PID controller is very unstable and/or sluggish. This is because the loop gain, which is the product of the controller and the process gain, can vary over several decades as the pH or the buffering changes. To try to alleviate this problem, Shinskey proposed a nonlinear function to compensate for the nonlinearity of the process. The function was a simple combination of three straight lines as shown in Figure 2-5. The deadband width and gain are adjustable to customize it to the neutralization function being controlled. These constants must be continually updated manually if the amount of buffering is changing with time. The function can be defined mathematically as

\[ f(e) = \text{sign}(e) \cdot \max(|e| - b, G_b |e|) \] (22)

where \( e \) is the pH error (set point - pH), \( b \) is half the width of the deadband and \( G_b \) is the gain within the deadband.

This characterized pH is used as the controlled variable in the PID controller instead of the actual pH, having the effect of lowering the controller gain around neutral to try to maintain a more uniform loop gain.

At very low buffering, it is impossible to properly fit the highly nonlinear pH function with this simple function.
Figure 2-5
Characterized pH function for the nonlinear PID
Also, this control scheme requires the independent adjustment of five interrelated control parameters (a difficult task, at best).

**Valve Characterization:** The use of equal-percentage valves introduces a gain variation with load which is undesirable. It is, therefore, necessary to compensate for this gain. Shinskey suggests the use of an analog divider which approximates the equal-percentage characteristics. For the purposes of this simulation, however, the nonlinearity was exactly reversed digitally. This could only be done approximately in a real system.

**Tuning of the Controller:** The tuning procedure outlined by Shinskey was followed for the most part in obtaining reasonable tuning parameters for each case. The procedure used is as listed:

1) set the derivative time to zero and the integral time to a very large value,
2) increase the controller gain until undamped oscillations are obtained,
3) set the deadband width slightly less than the amplitude of the oscillations,
4) set the derivative time equal to the period of oscillation divided by four times π,
5) set the integral time equal to the time constant of the controlled tank,
6) adjust the controller gain and the deadband gain until rapid, uniform damping is achieved.

The procedure used by Shinskey suggests a much shorter
integral time than that in step 5. It, however, was difficult to obtain stable control at low buffering with such a short integral time. An integral time approximately equal to the time constant of the control tank was found to provide the best control for this system.

Proposed Controller

As has been pointed out, the gain of a pH process varies greatly depending on the pH and on the buffering of the solution. This highly nonlinear gain makes conventional control schemes operate very inefficiently. This means there is a need to adjust the controller to these changes. If the changes are rapid, manual adjustments will not be enough to achieve satisfactory control. Ideally, the controller should adapt itself to the process it is controlling. In this case, the gain of the controller would have to change inversely with the changing process gain. The following is a development of a controller which does exactly that, adapts its gain to compensate for the changing process gain.

Simple Feedforward Model: If the logarithm of the reagent required for neutralization of a strong acid (no carbonate) is plotted against the pH of the incoming stream, a straight line is obtained for pH's outside of the neutral range. This is also approximately true for solutions which have the same relative amounts of strong and weak agents. These relationships can be seen in Figure 2-6 for a pH set
Figure 2-6
Moles of NaOH required to neutralize one liter of incoming solution to the set point (case for a set point of seven)
point of seven.

For an equal percentage valve, there is a linear relationship between the valve position, \( m \), and the logarithmic scale of the \( y \)-axis shown in Figure 2-6. (The two sequenced equal percentage valves drawn on this figure show the range of the valve position, zero to one.) This means that the linear relationship holds for the valve position versus incoming pH. The simple feedforward controller takes advantage of this linear relationship. Thus, the equation for the simple feedforward controller is as follows:

\[
m = m_0 + K_{ef} \cdot (r - \text{pH}_0)
\]  

(23)

where 
- \( m \) = output of controller
- \( m_0 \) = controller bias
- \( K_{ef} \) = feedforward gain
- \( r \) = pH set point
- \( \text{pH}_0 \) = incoming pH.

The controller bias, \( m_0 \), should be set to the value of the valve position which corresponds to the flow rate intercept for the system being controlled (i.e., \( m_0 \) for 10\(^{-7}\) mol NaOH is \(-0.767\)). The value for \( m_0 \) can be calculated from the system parameters for a given line in Figure 2-6 by the following formula:

\[
m_0 = \frac{\ln(M_0 F_{\text{in}} R / (F_{\text{vmax}} C_{\text{NaOH}}))}{\ln(R)}
\]  

(24)

where 
- \( M_0 \) = moles of NaOH at the intercept in Fig. 2-6
- \( F_{\text{in}} \) = inlet flow rate (l/s)
- \( F_{\text{vmax}} \) = maximum reagent flow


rate from the equal percentage valve (l/s)

\( C_{NaOH} = \text{concentration of the reagent (mol/l)} \)

\( R = \text{range of equal percentage valve (i.e., 1000).} \)

For the strong acid–strong base system, "\( M_0 \)" has the value of 10\(^{-7} \) moles of NaOH.

The feedforward gain, \( K_{ef} \), should be set to the slope of this same line (the change in "\( m \)" divided by the change in pH). The process gain, \( K_p \), is the reciprocal of this slope and is given by

\[
K_p = \frac{r - pH_0}{m - m_0}.
\]

(25)

If the degree of buffering changes appreciably, the process gain, \( K_p \), changes because of the change in the slope of the operating line. For a constant controller gain, \( K_{ef} \), the reagent delivery will be grossly in error. Therefore, systems utilizing this feedforward scheme require frequent manual adjustment of the feedforward gain to obtain satisfactory control. What is needed is for the process gain to be accurately estimated and automatically updated.

**Estimation of Process Gain:** The process gain can be estimated from the generalization of eq. (25) to yield

\[
K_p = \frac{pH_1 - pH_0}{m - m_0}
\]

(26)

where \( pH_1 \) is the pH after the reagent addition. This
estimation can best be achieved by utilizing an in-line controller (one in which there is a negligible lag caused by mixing between the point of reagent addition and the feedback probe) such as the one shown in Figure 2-7. Good mixing between the stream and the added reagent is essential and must be obtained by the use of an in-stream mixer which gives a high degree of mixing with a minimum of lag and dead time. A mixing tank between the reagent addition and the feedback probe would be undesirable because changes in the valve position would not directly and immediately affect the feedback value.

**Updating of Controller Gain:** The gain estimate obtained from this method is not exact. This is due to several factors such as probe noise and lag, dead time and lag between the probes, and valve dynamics. In other words, nothing in the equation is known exactly. These inaccuracies can and should be minimized by appropriate techniques (some of these will be discussed later).

Since each estimate incorporates these inaccuracies, substituting this process gain directly into the control equation would result in highly erratic behavior. To smooth this behavior, a digital filter can be used to exponentially update the estimate of the process gain used by the controller, such that

\[ K_p(n) = K_p(n-1) \cdot (1 - a_1) + R_p \cdot a_1 \]  \hspace{1cm} (27)

where \( a_1 \) = updating constant
Figure 2-7
In-line adaptive controller
The constant "a_i" should be adjusted to obtain a rapid, stable response to load changes.

Since "a_i" is equal to one minus the digital filtering constant, it can be expressed as

\[ a_i = 1 - \exp(-T/\tau_u) \]  \hspace{1cm} (28)

where \( T \) = sampling interval  (seconds)
\( \tau_u \) = updating time constant (seconds)

It may be useful, at times, to look at the tuning in terms of this time constant rather than the updating parameter. If the updating parameter is less than 0.1, the updating time constant is essentially the reciprocal of the updating parameter. This approximation provides a quick estimation of the time constant since most of the values of the updating constant are less than 0.1.

Summary of Adaptive Controller Algorithm: The equations for the adaptive algorithm were developed in the preceding pages. The procedure for implementation of the adaptive controller is 1) estimate the process gain, 2) average the process gain using a digital filter, and 3) use the reciprocal of this gain in the feedforward equation to obtain the controller output (valve position). These steps are executed at each sampling instant (for digital control). Mathematically, the procedure is as follows:
\[ K_p(n) = (pH_1(n) - pH_0(n))/(m(n-1) - m_0) \]  
\[ K_P(n) = K_P(n-1) \cdot (1 - a_1) + \hat{K}_P \cdot a_1 \]  
\[ m(n) = m_0 + (1/K_P(n)) \cdot (r - pH_0(n)) \].

An example of the gain updating procedure is given in Figure 2-8 for a ten-fold increase in the buffer concentration.

**Summary**

In this chapter, the mathematical models required for the simulation of the neutralization process, the NPID (standard) controller, and the adaptive controller were developed. Base values were given for the parameters defining the system (Marra, 1979). These base values are used in Chapter 3 to compare the stability and effectiveness of the adaptive controller to that of the NPID controller. Also discussed in Chapter 3 is the effect of the acid concentrations on the tuning limits of the adaptive controller.
Figure 2-8
Example of gain adaption for an ten-fold increase in carbonate concentration
(response for this case given in Figure 3-9)
CHAPTER III
RESPONSE AND STABILITY OF ADAPTIVE CONTROLLER

Introduction

In this chapter, the response and stability of the adaptive controller is compared to the nonlinear proportional-integral-derivative (NPID) controller for two cases: 1) a step change in the strong acid (HCl) concentration at various levels of buffering and 2) step changes in the weak acid (H₂CO₃) concentration. For these cases both controllers were tuned for optimal response to case 1. Next, the limits of acceptable response for the adaptive controller are correlated against strong and weak acid concentrations. Finally, the controllers are tested for response to a large step change in the concentrations of both the strong and weak acid (in the same direction).

Comparison of Nonlinear PID and Adaptive Controllers

Basis of Comparison: Figure 3-1 shows the configuration of the nonlinear PID controller. The nonlinear control loop is applied to the first tank. The second tank, which is uncontrolled, serves the purpose of averaging any oscillations leaving the first tank. This is essentially the configuration implemented by Shinskey in one of his
Figure 3-1
Shinskey's nonlinear PID control scheme
industrial applications (Shinskey, 1970). The time constants of the tanks and the associated dead times chosen for this study are two minutes and six seconds, respectively. These values are very close to those used by Shinskey in the above application, however, the tanks used are slightly smaller. This will have the effect of making the control a little more difficult.

In order to make comparisons between the controllers easier, the same flow configuration has been used for the adaptive control scheme. This control scheme is diagrammed in Figure 3-2. The main differences between the two configurations are the location of the control valve and the algorithm determining the position (opening) of the valve. The adaptive control scheme also requires an additional pH probe. The effect of changing the size of or removing the first tank in the adaptive control scheme will be discussed in Chapter 4.

For the cases studied, the inlet pH will always be acidic, requiring only the addition of NaOH. For a system in which the incoming pH can be acidic or basic, an identical control algorithm can be used to control a valve which adds HCl. The concepts developed are the same for both cases.

All of the cases in this chapter will be run with constant values for most of the parameters. These base values are summarized in Table 3-1.

Comparison of the Well-tuned Controllers: Figures 3-3
Figure 3-2
Adaptive feedforward control scheme
### TABLE 3-1

**Parameter values used in base cases**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>sampling interval</td>
<td>1</td>
<td>s</td>
</tr>
<tr>
<td>amplitude of noise in probes</td>
<td>±0.01</td>
<td>pH units</td>
</tr>
<tr>
<td>after mixed tanks</td>
<td></td>
<td></td>
</tr>
<tr>
<td>amplitude of noise in adaptive feedback probe, pH;</td>
<td>±0.1</td>
<td>pH units</td>
</tr>
<tr>
<td>probe lag</td>
<td>1</td>
<td>s</td>
</tr>
<tr>
<td>valve hysteresis (fraction of total valve movement)</td>
<td>0.005</td>
<td></td>
</tr>
<tr>
<td>valve lag</td>
<td>1</td>
<td>s</td>
</tr>
<tr>
<td>dead time between reagent addition and adaptive feedback probe, pH;</td>
<td>1</td>
<td>s</td>
</tr>
<tr>
<td>volume of tanks</td>
<td>120</td>
<td>l</td>
</tr>
<tr>
<td>inlet flow rate</td>
<td>1</td>
<td>l/s</td>
</tr>
<tr>
<td>dead time associated with tanks</td>
<td>5</td>
<td>%</td>
</tr>
<tr>
<td>(percent of tank retention time)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>adaptive feedforward intercept, m₀</td>
<td>-0.84</td>
<td></td>
</tr>
</tbody>
</table>
through 3-7 show the response of the well-tuned controllers at various levels of carbonate (buffer) concentration. Table 3-2 gives a brief description of the parameters listed in the legend.

The solid lines and the broken line on these graphs represent the measurements from the adaptive controller. Dotted lines (light and heavy) represent values from the NPID controller. The important quantities for comparison of the controllers are the pH values leaving each system. These are pH₂ (heavy solid line) for the adaptive controller and pHₐ (heavy dotted line) for the NPID controller. The other pH measurements, however, will also be presented to provide a better understanding of the behavior of each of the controllers.

Note, the carbonate concentrations above 0.0002 mol/l are only possible at slightly elevated CO₂ concentrations in the vapor and/or lower temperatures. This is because, in acidic solutions, the solubility of CO₂ in water is fairly low for normal atmospheric conditions. In basic solutions, the equilibrium shifts heavily toward HCO₃⁻ and CO₃²⁻, which greatly increases the total carbonates present in equilibrium with a given CO₂ vapor pressure.

From these figures, it can be seen that the adaptive controller (solid lines) gives tighter control than the NPID controller (dotted lines). Notice that, for this system, neither controller handles the case of zero buffering very well. The size of one or both tanks could be
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>adaptive updating parameter</td>
</tr>
<tr>
<td>KC</td>
<td>nonlinear PID controller gain</td>
</tr>
<tr>
<td>RESET TIME</td>
<td>NPID controller integral time, seconds</td>
</tr>
<tr>
<td>DERIV TIME</td>
<td>NPID controller derivative time, seconds</td>
</tr>
<tr>
<td>B</td>
<td>NPID controller deadband width, ±&quot;B&quot; pH units</td>
</tr>
<tr>
<td>GB</td>
<td>NPID controller deadband gain, fraction of controller gain</td>
</tr>
<tr>
<td>CL CONC</td>
<td>concentration of chloride ion in incoming stream, mol/l, before and after step change at time = 0</td>
</tr>
<tr>
<td>CARB CONC</td>
<td>total concentration of carbonates (carbonic acid + bicarbonate ion + carbonate ion) in incoming stream, mol/l, before and after step change at time = 0</td>
</tr>
<tr>
<td>INLET PH</td>
<td>incoming pH before and after step change at time = 0</td>
</tr>
<tr>
<td>PROBE NOISE</td>
<td>maximum amplitude of probe noise, pH units, for probes after a tank and the probe after the adaptive reagent addition, respectively</td>
</tr>
<tr>
<td>PROBE LAG</td>
<td>probe time constant, seconds</td>
</tr>
<tr>
<td>ND</td>
<td>dead time between adaptive probes (pH₀ and pH₁), seconds</td>
</tr>
<tr>
<td>VALVE HYST</td>
<td>valve hysteresis, fraction of full movement</td>
</tr>
<tr>
<td>VALVE LAG</td>
<td>valve time constant, seconds</td>
</tr>
</tbody>
</table>

**TABLE 3-2**

Description of parameters in pH versus time legend
Figure 3-3
Well-tuned controller responses for a carbonate concentration of $10^{-2}$ mol/l
Figure 3-4
Well-tuned controller responses
for a carbonate concentration of $10^{-5}$ mol/l
Figure 3-5
Well-tuned controller responses for a carbonate concentration of $10^{-4}$ mol/l
Figure 3-6

Well-tuned controller responses for a carbonate concentration of $10^{-5}$ mol/l
Figure 3-7
Well-tuned controller responses for no carbonate
increased to improve this situation. Fortunately, a totally unbuffered system is rare in industry.

If one looks at Figure 3-6 or 3-7, it first appears that the large changes in pH are caused by substantial changes in the valve position. However, this is not the case as is illustrated by Figure 3-8 (valve position for case shown in Figure 3-6). This figure shows that the valve position is very stable for the adaptive controller (more so than the NPID). The question is then: what causes these large, erratic oscillations? The answer lies in the fact that this is an in-line controller (no axial mixing between the reagent addition and the feedback measurement), therefore small errors in the valve position create much larger errors in the resultant pH. These oscillations are not very important, however, unless they are not damped out in the averaging tank (as in the case shown in Figure 3-7).

A great deal about the two controllers can be learned by studying Figure 3-6 and its associated valve position graph (Figure 3-8). The near-vertical changes in pH for the adaptive case are caused by small valve movements (the valve remains stationary for most of the time because of valve hysteresis). The more gradual decreases in pH are caused because the load coming into the adaptive controller is increasing with time (the first tank creates a lag in the step change). Note that the slope of these changes decreases as the output of the first tank lines out.

For the NPID controller, the series of oscillations
Figure 3-8
Valve position for a carbonate concentration of $10^{-6}$ mol/l
in Figure 3-6 between the times of 30 and 300 seconds are caused by the imperfect fit of the characteristic pH function to the actual titration curve. This high gain area is an indication of the nonconstant loop gain which could not be accurately characterized with the nonlinear function.

The valve movement for the NPID controller is slightly more oscillatory than that of the adaptive controller. Notice, also, that the NPID valve moves more rapidly to the new position. This is because the NPID controller must control the whole tank, whereas the adaptive controller only needs to increase the valve position to handle the more gradual change in load experienced at the first pH probe.

Out-of-tune Controllers: It has been shown that the adaptive controller can be tuned to handle a wide range of buffering at least as well as, if not better than, the NPID controller. How, then, do the two controllers behave if the buffering is changed with the tuning constants held constant? Figures 3-9 and 3-10 show an increase and a decrease of buffer concentration (from that of Figure 3-4), respectively, by a factor of ten.

For the increase in buffer concentration (Figure 3-9), both controllers respond more slowly than their well-tuned counterparts. The adaptive control scheme, however, returns to the set point much more rapidly than the NPID controller. The valve movement for both of these cases is fairly smooth.

On decreasing the buffer concentration (Figure 3-10), a more dramatic effect is observed. The adaptive controller
Figure 3-9
Response of controllers to an ten-fold increase in the buffer concentration (10^{-3} to 10^{-2} mol/l)
a) Valve position versus time

b) pH versus time

Figure 3-10
Response of controllers to a ten-fold decrease in the buffer concentration (10^-3 to 10^-4 mol/l)
handles the step change with very little deviation from set point (0.1 pH units) and a very smooth valve movement (Figure 3-10). By contrast, the NPID becomes very oscillatory and unstable after just a couple of minutes (one time constant of the tank). The valve cycling evident in Figure 3-10 for the NPID (dotted line) is highly undesirable since it is detrimental to the valve. It is also interesting to note that appreciable valve cycling was occurring even when the control seemed perfectly stable. This is due to the damping by the control tank which can mask large valve movements in the NPID control scheme. This condition is highly undesirable even if the pH stays within the allowable range. Valve cycling is more likely to occur with the NPID controller because the outlet pH is relatively insensitive to valve movements as compared to the adaptive controller. Also, since the NPID is more sensitive to buffering changes and it is, therefore, more likely to become unstable or sluggish.

Stability Limits for the Adaptive Control Scheme

For a given system, if the updating parameter in the adaptive controller is too large, the response becomes so oscillatory that the response from the averaging tank drifts away from the set point and/or the valve begins to cycle. If, on the other hand, the updating parameter is lowered too far, the response becomes too sluggish, forcing the final pH out of the allowable range (after a load or gain change)
before bringing it back to set point. These are taken as the high and low limits of the updating parameter, respectively. Examples of each of these cases are shown in Figures 3-11 and 3-12 for a strong acid increase of half of a decade.

The acceptable range of the updating parameter ,"a_1"," is illustrated in Figure 3-13 for a wide range of buffer concentrations at a HCl concentration of 0.001 mol/l. The horizontal arrow shows the range of carbonate concentrations in which satisfactory control would be obtained if the updating parameter was set at 7 x 10^{-3}. In other words, if the carbonate concentration dropped below 1.5 x 10^{-4} mol/l at this HCl concentration (10^{-3} mol/l), the controller would require retuning. The vertical arrow shows the range of updating parameters which would yield satisfactory control for a carbonate concentration of 10^{-3} mol/l (and an HCl concentration of 10^{-3} mol/l). The asymptotes for low buffering were obtained by runs with no carbonate.

**Effect of Strong Acid Concentration on Stability Limits:** Figure 3-14 shows the effect which the strong acid (HCl) concentration has on the upper and lower limits of the constant "a_1". It is obvious that, for the most part, a lower updating parameter (slower gain updating) is required for lower buffer concentrations. However, notice that the lower limit curves all pass through maximums. This occurs, in each case, when the carbonate concentration is approximately three times the HCl concentration. This is
Figure 3-11
Example of upper limit of adaptive controller stability
a) valve position versus time

b) pH versus time

Figure 3-12
Example of lower limit of adaptive controller stability
Figure 3-13
Range of acceptable updating constants for an HCl concentration of $10^{-3}$ mol/l
Figure 3-14
Plot of upper and lower limits of updating constant versus carbonate concentration
the range of concentration ratios in which the slope of the pH versus "reagent required" line changes from strong acid dominant to weak acid dominant. In other words, a strong acid step change effects a substantial change in the feedforward gain for the system. At the low updating parameters, the gain is not corrected rapidly enough and the pH drifts out of the acceptable range. The shift of the upper limit to higher asymptote at high buffer concentrations reflects the greater stability of these systems.

Generalized Stability Limits: Since the curves in Figure 3-14 appear to be approximately parallel, it is logical to try to generalize all of them into one pair of curves. Figure 3-15 shows the acceptable range for "a₁" versus the ratio of carbonate to hydrochloric acid concentration, a dimensionless quantity. The fit of the data to a single pair of curves is fairly good at the higher levels of buffering. At the lower levels of buffering, however, the curves do not fall on the same lines. The higher HCl concentrations are less stable at low buffering. This is because, at the low buffering, the gain around neutral is very high. The process is, therefore, much more sensitive to errors in the valve position. At the higher HCl concentrations, the valve is opened considerably more, and the error caused by valve hysteresis creates larger errors in the flow. This, in turn, causes larger oscillations in pH and therefore acceptable control is more
Figure 3-15
Plot of upper and lower limits of updating constant versus dimensionless buffer concentration
difficult or impossible to obtain. (The small inconsistencies in the plotted points can be explained by the fact that the feedforward intercept, \( m_0 \), is not the exact intercept of the feedforward lines.)

Response to Dilution: The generalized curves indicate that if the strong and weak acid concentrations are reduced by the same factor (the ratio remains constant), a well-tuned controller should remain well-tuned. This can be seen very graphically in Figure 3-16. Note also that by maintaining a constant ratio, the feedforward gain remains approximately constant. This is the reason why the disturbance from set point is minimal. The response obtained from the NPID controller for this step change is totally unacceptable and will require substantial changes in the tuning constants to bring it back to a stable operating point.

Summary

It was shown that the adaptive controller responded significantly better to a step change in the strong acid (HCl) concentration than the NPID controller at moderate to low buffer concentrations and approximately the same at high concentrations. When the buffer concentration was increased and decreased by a factor of ten, the NPID controller became sluggish and unstable, respectively. The adaptive controller, on the other hand, did not have these problems for changes in the buffer concentration. Also of importance
a) valve position versus time

b) pH versus time

Figure 3-16
Response of controllers to dilution
(both acid concentrations reduced by a factor of 50)
was the observed tendency of the NPID controller to cause valve cycling even with what appeared to be a stable response. This valve cycling is highly undesirable as it greatly reduces the life of the valve.

The stability of the adaptive controller was correlated versus strong and weak acid concentrations. It was found that these curves could be generalized into a single pair of curves by plotting the updating parameter against the ratio of the acid concentrations (a dimensionless quantity). This indicated that tuning should remain constant when the ratio of the strong and weak acid concentrations are maintained in the same ratio. This was illustrated by the stable response to a drop in both acid concentrations by a factor of fifty. This response was in stark contrast with the highly unstable response of the NPID controller.

It should also be noted that the NPID (five tuning constants) required considerably more time and effort to tune than did the adaptive controller (two tuning constants). This is very important if process changes occur frequently which necessitate retuning.

Chapter 4 will detail the sensitivity of the response and stability limits of the adaptive controller to pH probe noise and lag, valve hysteresis and lag and dead time between the adaptive pH probes. Also the effect of the enlargement or removal of the initial tank in the adaptive control scheme and the sensitivity of the control to the tuning constant “m0” will be investigated.
CHAPTER IV
PARAMETER SENSITIVITY ANALYSIS
FOR THE ADAPTIVE CONTROLLER

Introduction

In the previous chapter, the characteristics of the adaptive controller were investigated for constant values of several parameters (probe noise and lag, valve hysteresis and lag, dead time between the adaptive probes, tank volumes, inlet flow rate and feedforward intercept). It is important to know how the characteristics of the controller are affected by different values of these parameters. To this end, this chapter will illustrate the sensitivity of the controller to changes in each of these parameters. (The base values of all of these parameters are given in Table 3-1).

The values of interest are those relating to the probe and valve dynamics, dead time between the pH probes, and the initial tank volume. Also investigated will be the relaxation of certain assumptions such as constant flow rate and linear probe lag. Also, the sensitivity of the controller to the tuning parameter, \( m_0 \), which has been held constant for all of the previous cases will be discussed.

Each of the parameters will be tested at a value significantly above and below that used in the base cases.
shown in Chapter 3. For each of these cases, the well-tuned controller response will be given (to be compared to Figure 3-5). Also, for each case, the limits of acceptable tuning will be shown and any changes in these limits will be discussed. (Note: the dashed lines in the tuning limit graphs are the limits of the base case shown in Figure 3-13).

**Probe Dynamics**

As discussed in Chapter 2, the pH probe dynamics were modeled with a first order lag and uniformly distributed random noise. This section will first show the effect of different amplitudes of noise in each of the two different probes on the control performance. Next, the effect of different values of the probe lag will be illustrated. Finally, the assumption of a linear probe lag will be relaxed to allow for a different time constant when the pH is moving toward and away from neutral. The effect of the relaxation of this assumption will be discussed.

**Probe Noise:** There will probably be less complete mixing before the feedback probe for the adaptive controller, pH₁, than before the two probes immediately after the mixed tanks (the noise was considered to be a combination of incomplete mixing and electronic noise). Because of this, a separate (and, in general, higher) value of noise was used for this probe. The effect of higher and lower values of the noise levels in each of these probes is
illustrated below, starting with the probes immediately following the mixing tanks.

Figure 4-1 shows the well-tuned response of the controllers for no noise in the first probe. While the nonlinear proportional-integral-derivative (NPID) controller response was not significantly affected, the response of the adaptive controller is markedly smoother for this case. Figure 4-2 illustrates the effect which the lower noise level has on the limits of acceptable control for the adaptive controller. It is obvious from this graph, that the acceptable range has been greatly expanded. Most noteworthy is the improved control at low buffer concentrations.

On the other hand, it can be seen from Figure 4-3, that the controller response for a high amplitude of noise in the first probe (±0.03 pH units) is highly erratic. It should also be noted that a small, permanent offset (approximately 0.2 pH units) occurs for this higher amplitude of noise. The valve movement for both controllers (especially the adaptive controller) is more erratic. Figure 4-4 shows that the high (stability) limit of the adaptive controller is reduced and acceptable control cannot be achieved at low levels of buffering.

The adaptive control response is not affected noticeably by the reduction of the noise in the second probe to zero. This is also the case for the limits of acceptable control. The NPID controller is not affected at all by the
Figure 4-1
Controller response for no noise in the first probe
Figure 4-2
Tuning limits for no noise in the first probe

oscillatory

sluggish

gain updating parameter  
\( a_1 \)

HCl concentration
1.0 \( \times 10^{-3} \) (mol/l)

carbonate concentration (mol/l)
Figure 4-3
Controller response for noise of 0.03 pH units in the first probe
Figure 4-4
Tuning limits for 0.03 pH units of noise in the first probe
level of this noise since this probe is only found in the adaptive control scheme. For the case of higher noise (±1 pH unit) shown in Figure 4-5, the control is slightly more erratic, but the final pH remains very close to the set point. The limits of the tuning constant are illustrated in Figure 4-6. The stability limit of the tuning constant, $c_t$, is lowered substantially as compared to the base case at high levels of buffering. This is because, at the high values of updating, the high levels of noise have a very detrimental effect on the calculated gain of the controller.

As was shown, the noise in the second probe has considerably less effect on the control, even though much higher noise levels are present. This is because the second pH value only enters the control through the estimation of the gain. Since this gain is heavily filtered by the gain updating procedure (time constants for updating range from 10 to 10,000 seconds), the effective noise is significantly reduced. The noise in the first probe, however, enters both through the gain estimation and directly in the feedforward equation. This direct entry of the noise into the control equation means that even low levels of this noise have a relatively large effect on the controller output.

The relatively high sensitivity of the adaptive control to the noise in the first (feedforward) probe dictates that the level of this noise be kept as low as possible. This can be done by either analog or digital filtering. Since the frequency of the noise is probably fairly high, analog
a) valve position versus time

b) pH versus time

Figure 4-5
Controller response for 1.0 pH unit of noise in the second probe
Figure 4-6
Tuning limits for 1.0 pH unit of noise in the second probe
filtering would yield considerably more amplitude reduction for the same time constant (unless the sampling frequency is very high) and would therefore be preferable. Because the digital lag will be much larger unless the filter time constant becomes sufficiently large (larger than the dead time between the probes), the second probe can lead the first probe. This has a very detrimental effect on the gain estimation and the resultant control. Therefore, if filtering of the feedforward probe measurement is done, it would be preferable to only filter the measurement used in the feedforward formula and to use the unfiltered measurement in the gain updating. This is a very simple task if the filtering is done digitally.

**Probe Lag:** The effect of different values of the linear probe lag will be presented first and then a case showing the effect of a nonlinear lag will be shown. (Note: the same probe lag is used for all of the probes).

The control with no pH probe lag does not differ noticeably from the base case (one-second lag) shown in Chapter 3. The limits of acceptable control are also changed only slightly for this case. The response for a high probe lag (Figure 4-7), however, is considerably more sluggish than the base case for both control schemes. This is to be expected since the controllers do not receive the information needed to make the adjustments in the valve position as quickly. The limits of acceptable control for the adaptive controller (Figure 4-8) are affected
Figure 4-7
Controller response for a probe lag of 10 seconds
Figure 4-8
Tuning limits for a probe lag of 10 seconds
significantly by the increase in the lag. The high limit is reduced and the acceptable range for buffer concentrations below $3 \times 10^{-8}$ mol/l is lost. Low frequency oscillations (approximately 0.05 Hz) occur at the higher values of the updating parameter. This is due to the phase lag between the value of the pH measurements and the valve settings used in the gain estimation. This phase lag is caused by the large pH probe lag.

As noted earlier, some studies have indicated that the probe lag is nonlinear. It has been shown that the time constant of the probe when the pH is approaching neutral is approximately half the time constant moving away from neutral. For the case of a one second lag moving toward neutral and a two second lag moving away from neutral, the response is essentially the same as for a one second linear lag. The limits of acceptable tuning do not change appreciably for this case, either. The response and limits are changed very little from the ten second lag response if a lag of 6.5 seconds toward and twice this value away from neutral is used (this combination has an average lag of about ten seconds). These two cases show that the linear probe lag assumption is acceptable for reasonable values of this lag.

**Valve Dynamics**

As discussed in Chapter 2, the valves in this simulation incorporate both hysteresis (valve sticking) and
a first order lag. The effect of each of these nonlinearities will be studied in this section.

**Valve Hysteresis:** In Chapter 3, the valve hysteresis was held constant at 0.005 (0.5\% of the total valve movement). Since two valves are sequenced for this control scheme, each valve only acts over approximately half of the total valve movement. This means that the actual hysteresis for a given valve is roughly twice the stated value of 1\% for each valve. The hysteresis of a given valve can be affected by the age and lubrication of the valve and the gain of the valve positioner (as discussed in Chapter 2). The effect of different levels of this very nonlinear phenomenon on the controller performance is given below.

A well-tuned response for the case of no valve hysteresis is presented in Figure 4-9. The pH measurement at the first probe of the adaptive controller is considerably more erratic for this case than for the base case (Figure 3-5). The valve hysteresis in the base case acted as a nonlinear filter, reducing the effective noise in the system. With no hysteresis, the valve is much more responsive and therefore reacts more readily to inaccuracies in the calculations (mainly pH measurement noise). The response of the NPID controller is not affected noticeably by this reduction in the valve hysteresis. This is due to the fact that inaccuracies in the valve position are damped out effectively by the first mixing tank in this control scheme. The high limit of the updating parameter is reduced
Figure 4-9
Controller response for no valve hysteresis
slightly (Figure 4-10) because of the increased feedback of noise in the loop. This is also the reason that the control is degraded in the region of low buffering where accurate valve position is crucial.

For the case of a high value of hysteresis shown in Figure 4-11 (2% of total, or 3.5% of each valve), the adaptive control is seen to be considerably more sluggish, but fairly stable. The sluggish response is caused by the fact that valve does not respond until the controller output changes by two percent of the full range. The stability limit for this case (Figure 4-12) is reduced at moderate levels of buffering. The acceptable range at low levels is significantly narrower because of the problem with valve positioning. The low limit is actually improved (lowered) at mild levels of buffering for this value of hysteresis. This limit is improved because the amount of reagent required does not change much for the step in this range. The increased hysteresis keeps the controller from making a large initial correction for the change in the incoming pH before the gain is adjusted.

It appears then that a small amount of hysteresis is beneficial for the adaptive controller, while large amounts degrade the controllability of the loop. The NPID control loop is also affected by large values of hysteresis. In practice, all valves will have a certain degree of hysteresis. The degree of this hysteresis will depend on the valve and the positioner gain.
Figure 4-10
Tuning limits for no valve hysteresis

oscillatory

HCl concentration
1.0x10^-3 (mol/l)

sluggish

carbonate concentration (mol/l)
Figure 4-11
Controller response for a valve hysteresis of 2%
Figure 4-12
Tuning limits for a valve hysteresis of 2%

- Oscillatory
- Sluggish

HCl concentration
1.0x10^{-3} (mol/l)

Gain updating parameter \( (\alpha_1) \)

Carbonate concentration (mol/l)
Valve Lag: Since valves have a certain amount of inertia, a move to a new valve position will take a finite amount of time. This move is approximately a first order lag. The average time constant for a valve is about one second (this was the value used in the base runs in Chapter 3). The effect of no valve lag and a lag of ten seconds on the responses of the two controllers is discussed below.

The reduction of the valve lag to zero does not have much effect on either control response. This indicates that the valve lag of one second is not a large factor in the control of the base case. The limits of acceptable control for the adaptive controller are also essentially the same as for the base case.

Figure 4-13 shows the response of the two controllers for a valve lag of ten seconds. Both controllers are affected by the increase in the valve lag. The response for both is considerably more sluggish and the oscillations are of a lower frequency than for the one second time constant. The slow valve movement can cause the adaptive control to drift outside of the acceptable pH range on the initial step. This is the reason acceptable control is limited to higher levels of buffering (Figure 4-14). The increased valve lag creates a phase shift between the controller output to the valve and the pH measurements used in the gain estimation. This lowers the upper limit of the tuning constant because the gain estimate is not accurate enough for the high updating rates. At the lower buffer
Controller response for a valve lag of 10 seconds
Figure 4-14
Tuning limits for a valve lag of 10 seconds
concentrations, the valve does not react quickly enough to keep the pH in the acceptable range, eliminating the acceptable tuning for this region.

Dead Time

In the adaptive control scheme, a finite amount of time is required for the fluid to pass from the feedforward probe, pH₀, to the feedback probe, pHᵢ. This time has been modeled as a pure dead time (plug flow) of an integral number of sample times. Theoretically, this dead time should be zero for the rigorous calculation of the process gain. For the base cases presented in Chapter 3, the dead time was set at one second. The effect of dead times of zero and ten seconds are discussed below. Since this dead time is not part of the NPID control scheme, changes in this parameter do not affect its performance.

For the case of zero dead time, there was no noticeable change in the response from the base case shown in Figure 3-5. The acceptable range has been increased for the tuning of the adaptive controller. Most noticeable is the increase in the high limit at high levels of buffering (Figure 4-15). This is probably due to the fact that, with no dead time, the values for controller output (m) and the pH's before and after the reagent addition are more in phase. Since this provides a better point estimate of the gain, higher values of gain updating are acceptable. At unstable tuning values (too high) the output of the adaptive controller oscillates
Figure 4-15
Tuning limits for no dead time between the adaptive probes
at very high frequencies. This is because a change in the valve setting is felt almost immediately at the feedback probe for the case of no dead time.

If the dead time is increased to ten seconds (Figure 4-16), the control response is much slower and the gain updating constant must be much lower to provide stable control. For this value of dead time, effects of changes in the controller output are not detected for a relatively long time period. As can be seen from Figure 4-17, the acceptable range of tuning is severely limited by this level of dead time. The high limit of the updating parameter is dropped substantially. Phase lag in the estimation is very prominent because the feedback pH measurement used in this calculation relates to an inlet pH and controller output of about ten seconds before. High levels of updating are therefore very unstable. Tuning in this range results in large oscillations at relatively low frequencies.

Effective dead time has a fairly large impact on the controllability of the adaptive control scheme. This is due to the role it plays in the estimation of the gain used in updating. (Note: a filter could be added to the feedforward gain to compensate for the dead time between the probes and reduce the phase lag in the gain calculation. However, experience with this technique indicated that the control becomes unstable if the feedback probe leads the feedforward probe. The technique appeared to create more problems than it solved and is therefore not very promising). It is
Controller response for a dead time of 10 seconds

Figure 4-16
Figure 4-17
Tuning limits for a dead time of 10 seconds
interesting to note that one of the most important factors in the controllability of the NPID or similar feedback schemes is the value of the dead time associated with the control tank. Steps must be taken to keep this to a minimum or control becomes impossible.

**Inlet Tank Volume**

In all of the previous cases, the initial tank volume has been fixed at 120 liters (approximately two minutes residence time) for both control schemes. The effect on the control responses of initial tank volumes of zero and 240 liters will be discussed in this section. Since the initial tank is an integral part of the NPID control scheme, it cannot be operated if the volume is reduced to zero. Therefore, for this case, the NPID tank volume will be left at the base condition (120 liters).

If the initial tank is removed (tank volume = 0), a step change is felt directly and immediately by the adaptive controller. The complete effect of the concentration change is experienced before the gain has a chance to make any adjustment to accommodate it. This results in a very large initial upset followed by rapid updating to try to bring the pH back to the set point, as evidenced by Figure 4-18. The response lines out fairly quickly in this case because the load at the adaptive controller does not change after the step change at time = 0. This is in contrast with the control using an initial tank since the tank provides an
a) valve position versus time

b) pH versus time

Figure 4-18
Controller response for no inlet tank
exponential decay in the concentration change for a step change input. In the absence of an initial tank to reduce the impact of the step change in gain, the gain updating must be more rapid to prevent the pH from leaving the acceptable range (especially at low levels of buffering). This is seen by the upward shift of the low limit in Figure 4-19.

The controller behavior for this case seems considerably better when it is remembered that only one tank is being used. The NPID control scheme utilizes two mixing tanks. If the adaptive controller was placed before the first tank in this physical setup, more smoothing would take place and a wider range of tuning would be acceptable than with only one tank.

Oscillations are reduced slightly by increasing the initial tank volume to 240 liters (Figure 4-20). The lower limit is improved slightly (Figure 4-21) due to the fact that the concentration (and therefore gain) changes entering the adaptive controller are more gradual. This additional tank capacity should provide a similar improvement if added to the second mixing tank. The control by the NPID loop was not changed appreciably.

Flow Rate Increase

Flow upsets or changes occur in wastewater treatment but are usually of a much smaller magnitude than concentration changes. Generally, flow upsets are smoothed
Figure 4-19
Tuning limits for no inlet tank
Figure 4-20
Controller response for an inlet tank of 240 liters
Figure 4-21
Tuning limits for an inlet tank of 240 liters
(or damped) by the increase or the decrease in the capacity of the tanks or transfer lines. The most difficult case to control would be that of a constant volume system (such as the one modeled for this simulation). In this case, a step change in the flow rate will yield a step change at the adaptive controller. Bearing in mind that this is an extreme case, the effect of a 20% flow increase will be analyzed.

The step change in flow results in a step change in the process gain at the adaptive controller (Figure 4-22). The pH out of the controller immediately drops and the gain is then corrected to bring the pH back to the set point. Since no other load changes are experienced, the control lines out fairly quickly. Figure 4-23 shows that the tuning limits for a flow change are similar to those obtained for a step change in the acid concentration. One notable difference is the reduced stability at low buffering. High gain around neutrality and the rapid process gain change at the controller combine to account for this difference. NPID control response is much better for this step because the fluid in the tank is initially neutral for this control scheme. This reduces the initial deviation from set point.

Control for this type of disturbance, although not as good as for concentration changes, is quite acceptable considering this is the worst possible case. Flow changes which are more gradual (i.e., if capacity changes occur) should be handled by the adaptive controller with a response
Figure 4-22
Controller response for a flow rate increase of 20%
Figure 4-23
Tuning limits for a flow rate increase of 20%
similar to concentration changes.

**Tuning Parameter, m₀**

The tuning parameter, m₀, is the intercept for the feedforward calculation and should be set to a value relatively close to the intercepts on the graph shown in Figure 2-3. The actual value of this intercept, however, depends on the amount of strong and weak acid, the inlet flow rate and the size and range of the control valves. The value of m₀ must then lie somewhere in the appropriate range of values for the specific system.

For the base system and no buffering, the intercept is constant for all concentrations of the strong acid. This intercept is \(-0.767\) for the base flow rate and the valve combination used (calculated from eq.(24) in Chapter 2). Base runs were made with m₀ held constant at \(-0.84\). Cases will be shown for values of m₀ which are 0.3 units above and below this base value and the effect of these changes will be discussed. The NPID control will, of course, not be affected by the value of this parameter since it is only used in the adaptive algorithm.

For the case of a higher intercept (Figure 4-24), the control is not as tight as that of the base case. The measurement at the adaptive feedback probe, pH₁, is slightly less erratic for this case (m₀ = \(-0.54\)). The low limit (Figure 4-25) for this case is improved (lowered) over the base case for mild levels of buffering but considerably
Figure 4-24
Controller response for $m_0 = -0.54$
Figure 4-25
Tuning limits for $m_0 = -0.54$
worse at low levels. This is because this intercept is slightly closer to the actual value at the moderate conditions but the intercept used in the base case is better for low buffering.

If an intercept of \(-1.14\) is used (Figure 4-26), larger oscillations in the output pH are observed. Also, the final pH reaches approximately 0.1 pH units above neutral before having been brought slowly back to the set point. The limits of acceptable tuning (Figure 4-27) are worse (narrower) at almost every level of buffering, mostly at low levels.

From these cases, it appears that the control is considerably more sensitive to the value of \(m_0\) at low levels of buffering than in the other ranges. This would seem to indicate that the value of \(m_0\) should be chosen to be as close as possible to the intercept for a strong acid (this can be calculated from eq.(24) in Chapter 2). Control at the higher buffer concentrations should only be affected slightly by this selection.

**Summary**

This chapter studied the effect on the response and stability of the adaptive control for values of the various parameters which were higher and lower than the base case values. Also studied was the effect of a nonlinear probe lag and a flow rate change. The most notable findings were as follows:
a) valve position versus time

b) pH versus time

Figure 4-26
Controller response for $m_o = -1.14$
Figure 4-27
Tuning limits for $w_0 = -1.14$
1. most of the erratic behavior was due to the influence of the first probe (pH₀) noise,

2. reduction of the noise in the first probe resulted in a significant improvement in control at low concentrations of buffer,

3. relatively stable control was achieved even at very high noise levels of the feedback probe, pH₁,

4. large values of probe or valve lag or dead time created a phase lag in the gain estimation which severely affected the upper limit of the gain updating parameter,

5. linear probe assumption is fairly good at reasonable values of probe lag,

6. a small amount of valve hysteresis is beneficial to the adaptive control because it acts as a nonlinear filter of probe noise,

7. acceptable control could be achieved without a mixing tank before the adaptive controller,

8. acceptable control could be obtained for a flow rate change, even for the worst case of no volume change,

9. the tuning limits are relatively insensitive to the value of the tuning parameter, m₀, at moderate to high buffer concentrations, allowing this parameter to be determined by the low buffering intercept.

One should not be misled by the fact that in most of the cases acceptable control was not obtained for the low concentrations of buffer. This would be a very difficult, if not impossible control for a single controller with such small averaging tanks. Remember the poor control obtained by the NPID controller at these low levels of buffering (Figures 3-7 and 3-8). Larger control tanks or a trim controller on the second tank would allow acceptable control
at these stringent conditions.

Valve lag and hysteresis should not be a problem if a valve positioner is used. The most important parameters for obtaining good adaptive control would be the noise at the first probe and the dead time between the probes. This is because the controller is more sensitive to these values than any of the other parameters. Also important at the lower limits of buffering is the selection of the feedforward intercept, \( m_0 \). As noted, this should be kept close to the intercept for a strong acid system.
CHAPTER V
CONCLUSIONS

The purpose of this research was to develop an adaptive feedforward controller which would be less sensitive to the large gain changes found in wastewater treatment, comparison of this controller to an advanced controller common in industry, and the study of the effect of various system parameters on the operation of the developed controller.

The well-tuned controllers both responded adequately for acid concentration at high level of buffering but the adaptive controller response was considerably tighter at the low buffer concentrations. The most notable difference between the controllers was the increased stability demonstrated by the adaptive controller over the NPID controller for step changes in the buffer concentration. The NPID controller became unstable when the buffer concentration was reduced by a factor of ten.

Two tuning constants were required for the adaptive controller. It was shown that one of these constants, the feedforward intercept, could be essentially left at the intercept for the strong acid (on a "reagent required vs. pH error" graph). This meant that the tuning of the controller could be maintained by adjusting only one constant, the gain updating parameter. On the other hand, the NPID controller
required the adjustment of five tuning constants. This proved to be a very difficult and time-consuming job. Difficulty in tuning is especially troublesome since the NPID controller tuning was shown to be more sensitive to the buffer concentration than the adaptive controller and therefore has to be retuned more frequently.

The NPID controller appeared to react quicker to changes in flow rate and was less sensitive to the noise present in the pH measurements. Unlike the NPID controller the adaptive controller became erratic at very low values of the valve hysteresis. However, these low values (below 1% of an individual valve movement) will probably never be encountered in industrial applications.

Another consideration is the assumption made in the mathematical neutralization model of instantaneous reactions. This assumption is acceptable in many applications but in some systems (i.e., solutions containing lime) one or more of the reaction rates are slow (requiring more than a second or two to go to completion). In these cases, the adaptive controller would be affected more than a control scheme incorporating a mixing tank between reagent addition and the feedback pH to allowing more time for the reactions to occur (such as the NPID controller). When one or more of the reactions are slow, the pH will be brought to the set point at the feedback probe but the pH will change with time after this point. Additional trim controlling would be required to then bring it back to set point.
The controllers were simulated digitally for the convenience of this research. However, the adaptive controller could be designed using either digital or analog components, as could the NPID controller.

The adaptive controller, under most conditions, provided superior control and improved stability over the NPID controller. Control using the adaptive controller should also be improved (over the NPID) since it is easier to keep it within acceptable tuning limits (requiring only two tuning constants). If care is taken in the design of the control surroundings to keep the system parameters in acceptable ranges (especially the first probe noise and the dead time between the probes) this controller should be easy to keep tuned and should provide improved controllability.

Additional study should be done on:

1) performance of the controller when the valve combination switches from the large to the small valve, or visa versa,

2) performance of the controller for mixtures of weak acids,

3) problems involved with having both acid and base reagent valves.

Laboratory or in-field testing of the digital simulation is necessary to determine where the simulation does not provide an acceptable fit to the actual system and to determine better values of the various parameters in the system.
NOMENCLATURE

**English**

- **a**: tank lag filtering constant
- **a_p**: pH probe lag filtering constant
- **a_i**: updating constant for adaptive controller
- **b**: half of deadband width in NPID controller, pH units
- **C_{nach}**: concentration of the reagent, mol/l
- **e**: pH error from setpoint, (setpoint - pH)
- **e(n)**: pH measurement error at sampling instant "n", pH units
- **e_{max}**: maximum pH measurement error, pH units
- **f(e)**: characterized pH function (NPID controller)
- **F**: flow rate, liters/sec
- **F_a**: force of air on valve diaphragm
- **F_in**: inlet flow rate, liters/s
- **F_f**: force of friction in valve
- **F_s**: force of spring in valve
- **F_v**: flow rate through valve, liters/sec
- **F_{vmax}**: maximum flow rate through valve, liters/sec
- **G_b**: gain in NPID deadband (as a fraction of the gain outside the deadband)
- **K_{b1}**: first weak acid dissociation constant
- **K_{b2}**: second weak acid dissociation constant
- **K_{ef}**: feedforward gain
\[ \begin{align*}
K_p & \quad \text{process gain} \\
K_p & \quad \text{point estimate of process gain} \\
K_p(n) & \quad \text{digital estimate (filtered) of process gain at sampling instant } n \\
K_v & \quad \text{gain of valve positioner} \\
K_w & \quad \text{water dissociation constant} \\
m & \quad \text{output signal from controller, (0 to 1)} \\
m_a & \quad \text{signal from controller, (0 to 1)} \\
m_0 & \quad \text{feedforward controller bias and adaptive controller constant} \\
m_x & \quad \text{valve position, (0 to 1)} \\
m_f & \quad \text{valve stem friction as a fraction of full movement} \\
M_0 & \quad \text{moles of NaOH required at the intercept of Fig. 2-6} \\
N_d & \quad \text{dead time/time step size} \\
pH_a & \quad \text{actual pH value, pH units} \\
pH_i & \quad \text{pH measurement at point } i, \text{ pH units} \\
pH(n) & \quad \text{lagged pH measurement without noise} \\
pH_i(n) & \quad \text{lagged pH measurement with noise (transmitted to controller)} \\
r & \quad \text{pH set point, pH units} \\
R & \quad \text{range of valve (max flow/min flow)} \\
t & \quad \text{time, seconds} \\
T & \quad \text{digital sampling interval, seconds} \\
w_{max} & \quad \text{amplitude of pH measurement noise, pH units} \\
w(n) & \quad \text{value of measurement error at sampling interval, } n \text{ (pH units)} \\
V & \quad \text{tank volume, liters} \\
x & \quad \text{concentration of chloride ion, mol/l}
\end{align*} \]
\[ y \] concentration of sodium ion, \text{mol/l} \\
\[ z \] total concentration of carbonate, \text{mol/l} \\
\[ ([H_2CO_3] + [HCO_3^-] + [CO_3^{2-}]) \]

\text{Greek}

\[ \Delta t \] integration time step, \text{seconds} \\
\[ \tau \] time constant, \text{seconds} \\
\[ \tau_p \] pH probe time constant, \text{seconds} \\
\[ \tau_u \] updating time constant, \text{seconds} \\
\[ \tau_v \] valve time constant, \text{seconds}
REFERENCES


11. Mellichamp, D. A. and D. R. Coughanowr and L. B.


APPENDIX A

PROGRAM LISTING
SIMULATION AND CONTROL OF EFFLUENT PH USING ADAPTIVE FEEDFORWARD

1. HYDROCHLORIC AND CARBONIC ACID SYSTEM NEUTRALIZED BY NAOH

2. NONLINEAR PROPORTIONAL-INTEGRAL-DERIVATIVE DEVELOPED BY F. G. SHINSKEY (1970)

3. ADAPTIVE CONTROLLER DEVELOPED BY RICHARD A. BALHOFF (1982)

IMPLICIT REAL*(A-H,O-Z)
DIMENSION CZ0$(100), NARUN(4), CNAWS(100), CZWS(100),
   CNA0S(100), CNA1S(100), CZ1S(100)

DATA ISEED/395738471/,
   D TIME, XMO, FLOW00, RANGE1/0.D0,-8.41D-1,1.D0,1.D3/,
   D MAX, CONCNA, R1/8.D-2,2.5D-1,7.D0/

--- READ IN RUN DATA ---

X1 = 1.D0

996 WRITE(4,98)
98 FORMAT( ' ENTER RUN # (4A4)' )
READ(5,99) NARUN
99 FORMAT(4A4)
995 WRITE(4,101)
101 FORMAT( ' ENTER FINAL TIME, TIME STEP, TANK VOLS(3),' ,
   F ' NOISE SDS' )
READ(5,*) FTIME, DT, V0, VA, V3, SD, SD2
994 WRITE(4,102)
102 FORMAT( ' ENTER PROBE LAG (SEC),' ,
   F ' VALVE HYSTERESIS AND LAG AND DEAD TIME' )
READ(5,*) TAUP, FRACH, TAUV, NI
993 WRITE(4,103)
103 FORMAT( ' ENTER INLET FLOW RATE (L/S),' ,
   F ' INTERCEPT (MO), AND NONLINEAR LAG RATIO' )
READ(5,*) FLOW0, XMO, RATIOL
992 WRITE(4,202)
202 FORMAT( ' ENTER INLET CL CONCS (FROM, TO),' ,
   F ' AND LENGTH OF PULSE' )
READ(5,*) CCL01, CCL00, NPUL
991 WRITE(4,203)
203 FORMAT( ' ENTER INLET CARBONATE CONCS (FROM, TO)' )
READ(5,*) CZ01, CZ00

900 CONTINUE

405 FORMAT( ' ENTER A1, KCPI, TIPI, DERIV TIME,' ,
   F ' DEADBAND WIDTH, DEADBAND GAIN, IGOTO' )
READ(5,*,END=999) A1, XKCP1, TIPI, TD, B, GB, IGOTO

C IF( A1.LT.0.D0 ) GOTO 999
C
C----------------SET UP CONSTANTS
C
ISEED = 395738471
CCL0 = CCL00
CZ0 = CZ00
ITMAX = FTIME/DT + 5.D-1
MDO = V0/2.D1 + 5.D-1
NDA = VA/2.D1 + 5.D-1
AV = 0.D0
IF( TAUU/DT.GT.2.D-2) AV = DEXP(-DT/TAUU)
AT0 = 0.D0
AP = 0.D0
AP2 = 0.D0
IF( V0.LE.0.D0 ) GOTO 81
IF( DT*FLOWO/V0.LT.5.D1 ) AT0 = DEXP(-DT*FLOWO/V0)
81 IF( TAUU/GT.2.D-2 ) AP = DEXP(-DT/TAUU)
IF( TAUU=RATION/DT.GT.2.D-2 )
ATD = 0.D0
IF( TD.GT.0.D0 ) ATD = DEXP(-DT=1.D1/TD)
C
C----------------INITIALIZE (TIME = 0-)
C
TIME = 0.DO
FNAOH1 = TITVOL( R1,-CCL0I*FLOW00, CZ0I*FLOW00,CONCNA )
IF( DABS<FNAOH1).LE.FMAX1/RANGE1 ) FNAOH1 = 0.DO
PH0I = PH( -CCL0I,CZ0I )
FLOW1 = FLOW00 + FNAOH1
CZ1 = CZ0I - FLOW00 / FLOW1
CNA1 = (FNAOH1*CONCNA - CCL0I*FLOW00) / FLOW1
CNATO = - CCL0I
CZTO = CZ0I
PHO = PH( -CCL0,CZ0 )
PHT0 = PH( CNATO,CZTO )
PH1I = PH( CNA1,CZ1 )
C
IF( FNAOH1.NE.0.DO )
I XM = (DLOG(FNAOH1) - DLOG(FMAX1)) / DLOG(RANGE1)
I + 1.DO
XMM = XM
XKP1 = (PH1I - PHT0) / (XM - XMO)
XMLM = XM
XMPI = RANGE1**((XM - 1.DO)
F = XMPI
FNAPI = FNAOH1
CNA1 = (FNAH1*CONCNA - FLOW00*CCL0I)/(FNAPI+FLOW00)
CZTW = CZ0I - FLOW00 / (FNAPI + FLOW00)
C
C----------------INITIALIZE TANKS (TIME = 0)
C
CNA2 = CNA1
CNA3 = CNA1
CZ2 = CZ1
CZ3 = CZ1
PH2 = PH1I
PHB = PH1I
PHA = PH1I
PHANLG = PHA

C
NO = 0
CALL DEADI( I4,CNATW,CNAWD,CNAWS,NDA,100 )
CALL DEADI( I5,CZTW,CZWD,CZWS,NDA,100 )
CALL DEADI( I6,CNA0T,CNA0D,CNA0S,NDA,100)
CALL DEADI( I7,CZT0,CZ0D,CZ0S,NDA,100 )
CALL DEADI( I8,CNA1,CNA1D,CNA1S,NDA,100 )
CALL DEADI( I9,CZ1,CZ1D,CZ1S,NDA,100 )

C
PH1 = PH( CNA1,CZ1 )
GAIN = 0.0
IF( XMPI.GT.1.D-20 ) GAIN = (PH1 - PH0) / XMPI
WRITE(4,*) GAIN

C
C-------------INITIAL WRITE STATEMENTS
C
ITMAX1 = ITMAX + 1
WRITE(1,*) ITMAX1
WRITE(1,15) NARUN, A1, XKCP1, B, TIP1, GB, TD,
W CCL01, CCL0, CZ01, CZ0, PH01, PH0,
W SD, SD2, TAUP, N1, FRAC, TAU
15 FORMAT(16X,4A4/
F 5X,'A1 ',G10.3/
F 5X,'KC ',G10.3', B ',G10.3/
F 5X,'RESET TIME ',G10.3', GB',G10.3/
F 5X,'DERIV TIME ',G10.3/
F 5X,'CL CONC ',G10.3', TO',G10.3/
F 5X,'CARB CONC ',G10.3', TO',G10.3/
F 5X,'INLET PH ',G10.3', TO',G10.3/
F 5X,'PROBE NOISE',G10.3,4X,G10.3/
F 5X,'PROBE LAG ',G10.3', ND',16/
F 5X,'VALVE HYST ',G10.3', LAG',G9.3//)

C
WRITE(4,25) PH01, PH0
25 FORMAT(/5X,'INLET PH ',G12.4', TO',G12.4/)

C
WRITE(1,35) TIME, PHTO, PH1, PHA, PH2, PHB, XM, XM
W ,XKP1, XKP1, XKP1
WRITE(6,35) TIME, PHTO, PH1, PHA, PH2, PHB, XM, XM
35 FORMAT(/6X,'TIME',5X,'PHOT',7X,'PH1',7X,'PHA',7X,
F 'PH2',7X,'PHB',8X,'XM',6X,'XMPI',
F //F10.2,7F10.3,3G15.6)

C
C------------------MODEL AND CONTROLLERS
C
DO 100 IT=1,ITMAX

C
TIME  = TIME + DT
FLOW1  = FLOW0 + FNAOH1
FLOW2  = FLOW1
FLOWA  = FLOW0 + FNAPI
FLOWB  = FLOWA

C-------------------AVERAGING TANK FOR NPID
C
ATB  = 0.D0
IF( DT*FLOWB/V3.LT.5.D1 ) ATB = DEXP( -DT*FLOWB/V3 )
CALL TANK( ATB,CNAWD,CZW0,CNA3,CZ3,PHBZ )
APO  = AP
IF( DABS(7.DO-PHB).GT.DABS(7.DO-PHBZ) ) APO = AP2
WRITE(6,*) APO,PHB,PHBZ

C-------------------AVERAGING TANK FOR ADAPTIVE CONTROLLER
C
AT2  = 0.D0
IF( DT*FLOW2/V3.LT.5.D1 ) AT2 = DEXP( -DT*FLOW2/V3 )
CALL TANK( AT2,CNA1D,CZ1D,CNA2,CZ2,PH2Z )
APO  = AP
IF( DABS(7.DO-PH2).GT.DABS(7.DO-PH2Z) ) APO = AP2
WRITE(6,*) APO,PH2,PH2Z

C-------------------SMOOTHING TANK BEFORE ADAPTIVE CONTROLLER
C
CNATO = CNATO*ATO - CCL0*(1.DO - ATO)
CZTO  = CZTO*ATO + CZO*(1.DO - ATO)
CALL DEADT( 16,CNATO,CNAOD,CNAOS,NDO,100 )
CALL DEADT( 17,CZTO,CZOD,CZOS,NDO,100 )
PHOZ  = PH( CNAOD,CZOD )
APO  = AP
IF( DABS(7.DO-PHTO).GT.DABS(7.DO-PHOZ) ) APO = AP2
WRITE(6,*) APO,PHTO,PHOZ

C-------------------NPID CONTROL TANK (STANDARD CONTROL)
C
ATA  = 0.D0
IF( VA.LE.0.DO ) GOTO 82
IF( DT*FLOWA/VA.LT.5.D1 ) ATA = DEXP( -DT*FLOWA/VA )
82 CNATWO = (FNAPI*CONCNA - FLOWO*CCL0) / (FNAPI+FLOWO)
CZWO  = CZ0 * FLOW0 / (FNAPI + FLOWO)
CALL TANK( ATA,CNATWO,CZWO,CNATW,CZT,W,PHS )
CALL DEADT( 14,CNATW,CNAWD,CNAWS,NDA,100 )
CALL DEADT( I5,CZTW,CZWD,CZWS,NDA,100 )
PHAZ = PH(CNAWD,CZWD)
APO = AP
IF( DABS(7.DO-PHA).GT.DABS(7.DO-PHAZ) ) APO = AP2
WRITE(6,*) APO,PHA,PHAZ
C
PHA = APO*PHA + (1.DO - APO)*PHAZ
WRITE(6,*) PHA
C
-------------ADAPTIVE FEEDFORWARD PROCESS CALCULATIONS

CNA1 = (FNAOH1=CONCNA + CNAOD*FLOWO) / FLOW1
CZ1 = CZOD = FLOWO / FLOW1
CALL DEADT( I8,CNA1,CNA1D,CNA1S,N1,100 )
CALL DEADT( I9,CZ1,CZ1D,CZ1S,N1,100 )
PH1Z = PH( CNA1D,CZ1D )
APO = AP
IF( DABS(7.DO-PH1).GT.DABS(7.DO-PH1Z) ) APO = AP2
WRITE(6,*) APO,PH1,PH1Z
C
WRITE(6,*) PH1
C
WNOIS2 = WNOIS(ISEED,SD2)
PH1N = PH1 + WNOIS2
C
-------------NONLINEAR PID CONTROLLER CALCULATIONS

ERRA = DABS(R1 - PHAN)
ERRC = DMAX1(ERRA-B, ERRA=GB)
IF( R1-PHAN.LT.O.DO ) ERRC = -ERRC
PHEFF = R1 - ERRC
XMPI = XKAPI*(ERRC + TD/DT*(PHANLG - PHEFF)) + F
PHANLG = PHANLG*ATD + PHEFF*(1.DO - ATD)
IF( XMPI.GT.1.DO ) XMPI = 1.DO
IF( XMPI.LT.0.DO ) XMPI = 0.DO
F = F + DT/TIPI*(XMPI - F)
C
"LINEARIZE" THE EQUAL PERCENTAGE VALVE

XML = 0.DO
IF( XMPI.GT.1.DO/RANGE1 )
    XM = DLOG(XMPI)/DLOG(RANGE1) + 1.DO
C
CALL VALVE( FRACH,AV,XML,XLM )
FNAPI = FMAX1*RANGE1***(XMLM - 1.DO)
C
-------------ADAPTIVE CONTROLLER CALCULATIONS

IF( XM-XMO.0.DO ) XKPIE = (PH1N - PHON)/(XM-XMO)
XKP1F = XKPIE
IF( XM.NE.0.DO ) XKPI =
    0 XKPIE*A1 + XKPI*(1.DO - A1)
XM = XMO + (R1 - PHON)/XKP1
C
IF( XM.GT.1.DO ) XM = 1.DO
IF( XM.LT.0.D0 ) XM = 0.D0

CALL VALVE( FRACH,AV,XM,XMM )
FNAOH1 = FMAX1*RANGE1**(XMM - 1.D0)
IF( XM.LE.0.D0 ) FNAOH1 = 0.D0

C-----------------CALCULATE ACTUAL PROCESS GAIN

FNAA = TITVOL( R1,CNAOD,CZOD,CONCNA )
XMA = (DLOG(FNAA) - DLOG(FMAX1))/DLOG(RANGE1) + 1.D0
XKP1A = (R1 - PHT0) / (XMA - XMO)

C-----------------END PULSE

IF( IT.EQ.NPUL ) CCL0 = CCL0I
IF( IT.EQ.NPUL ) CZ0 = CZ0I

C------------------WRITE STATEMENTS

WRITE(1,205) TIME, PHOZ, PH1Z, PHAZ, PHZZ, PHBZ,
W XMM, XMLM,XKP1A, XKP1F, XKP1
WRITE(6,205) TIME, PHOZ, PH1Z, PHAZ, PHZZ, PHBZ,
W XMM, XMLM
205 FORMAT(F10.2,7F10.3,3G15.6)

C 100 CONTINUE
GOTO(991,992,993,994,995,996),IGOTO

C GOTO 900

C 999 RETURN
END
FUNCTION PH( CNA, CZ )

FINDS PH OF STREAM BY INTEGRAL HALVING
FOLLOWED BY NEWTON'S METHOD

CNA – (CONCENTRATION OF NAOH -
CONCENTRATION OF HCL), MOL/L

CZ – TOTAL CONCENTRATION OF CARBONATES,
MOL/L

IMPLICIT REAL*8(A-H,O-Z)
PH = 7.DO
N = 20
PH1 = 0.DO
F1 = FUNC(PH1, CNA, CZ)
PH2 = 14.
F2 = FUNC(PH2, CNA, CZ)
DO 200 I=1,N
PH3 = (PH2 + PH1) / 2.DO
F3 = FUNC(PH3, CNA, CZ)
IF( F1*F3.GT.0.DO ) GOTO 50
PH2 = PH3
F2 = F3
GOTO 200
50 IF( F2*F3.GT.0.DO ) GOTO 60
PH1 = PH3
F1 = F3
200 CONTINUE
PH = PH1 - F1*(PH2-PH1)/(F2-F1)
RETURN
60 WRITE(6,15) TIME
15 FORMAT('0**** PH ROOT NOT FOUND AT',F10.2,' SEC')
RETURN
END
FUNCTION FUNC( PH, CNA, CZ )

TRIAL AND ERROR FUNCTION FOR PH CALCULATION
FOR CARBONIC ACID, HCL, AND NAOH SYSTEM

EQUILIBRIUM CONSTANTS (XKB1 AND XKB2)
ARE FOR CARBONIC ACID

IMPLICIT REAL*8(A-H,O-Z)
DATA XKW, XKB1, XKB2 /1.D-14, 4.467D-7, 5.61D-11/

H = 1.D1 ** (-PH)
FUNC = (((H + CNA + XKB1)**H + XKB1*(CNA - CZ) - XKW
F + XKB1*XKB2)
F **H + XKB1*XKB2*(CNA - 2.D0*CZ) - XKW*XKB1)**H
F - XKW*XKB1*XKB2
RETURN
END
FUNCTION TITVOL( PH, CNA, CZ, CNAOH )

CALCULATES THE VOLUME OF NAOH REQUIRED TO
NEUTRALIZE A SOLUTION TO "PH"

PH — FINAL PH OF SOLUTION
CNA — (CONC OF NAOH — CONC OF HCL), MOL/L
CZ — TOTAL CONC OF CARBONATES, MOL/L
CNAOH — CONC OF NAOH ADDED (REAGENT), MOL/L

IMPLICIT REAL*8(A-H, O-Z)
DATA XKW, XKB1, XKB2 /1.D-14, 4.467D-7, 5.61D-11/

C
H = 1.D1 ** (-PH)
C = H - XKW/H
XKB11 = XKB1/H
XKB22 = XKB2/H
SUM = 1.DO + XKB11 + XKB11*XKB22

C
FRAC = (XKB11 - XKB22*XKB11**2/SUM)/(1.DO + XKB11)
F = 2.DO*XKB11*XKB22/SUM
TITVOL = (CZ*FRAC - CNA - C) / (CNAOH + C)

C
RETURN
END
SUBROUTINE DEADT( I, X, XD, XS, N, NMAX )

PURPOSE - TO DELAY AN INPUT X BY N CALLS

I INDEX
X INPUT
XD OUTPUT (DELAYED INPUT)
XS(NMAX) STORAGE STACK
N NO. OF DEADTIMES
NMAX MAXIMUM NO. OF DEADTIMES + 1

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION XS(NMAX)

IF( N.GE.NMAX ) N = NMAX - 1
IF( N.LE.0 ) N = 0

XS(I) = X
ID = I - N
IF( ID.LE.0 ) ID = ID + NMAX
XD = XS(ID)
I = I + 1
IF( I.GT.NMAX ) I = 1
RETURN

INITIALIZATION

ENTRY DEADI( I, X, XD, XS, N, NMAX )

DO 10 I=1,NMAX
10 XS(I) = X
XD = X
I=1
RETURN
END
SUBROUTINE TANK( A,CNAI,CZI,CNA,CZ,PHO )

PURPOSE - TO SIMULATE A FIRST ORDER LAG
(MIXED TANK)

A       LAG CONST (DEXP(-DT/V))
CNAI    CONC OF NA INPUT TO TANK
CZI     CONC OF Z INPUT TO TANK
CNA     CONC OF NA AT OUTPUT OF TANK
CZ      CONC OF Z AT OUTPUT OF TANK
PHO     PH AT OUTPUT OF TANK

IMPLICIT REAL*8(A-H,O-Z)

CNA   = CNA*A + CNAI*(1.DO - A)
CZ    = CZ*A + CZI*(1.DO - A)
PHO   = PH(CNA,CZ)

RETURN
END
SUBROUTINE VALVE( FRAC, A, XM, XMM )

PURPOSE - TO SIMULATE HYSTERESIS AND LAG IN A CONTROL VALVE

FRAC - FRACTION OF VALVE POSITION FOR HYSTERESIS
A - LAG CONST (EXP(-T/TAU))
XM - VALVE POSITION FROM CONTROLLER
XMM - ACTUAL VALVE POSITION (OUTPUT)

IMPLICIT REAL*8(A-H,O-Z)

DIFF = XM - XMM
DIFF1 = DABS(DIFF) - FRAC
IF( DIFF1.LT.0.DO ) DIFF1 = 0.DO

DIFF2 = 0.DO
IF( DIFF.NE.0.DO ) DIFF2 = DIFF1 * DIFF / DABS(DIFF)
XMI = XMM + DIFF2

XMM = XMM*A + XMI*(1.DO - A)
WRITE(6,* ) XMI, XMM

RETURN
END
FUNCTION WNOIS(ISEED, SD)

PURPOSE - TO CALCULATE UNIFORMLY DISTRIBUTED RANDOM NOISE WITH A MAXIMUM ABSOLUTE VALUE OF SD. ISEED IS THE SEED FOR SUBROUTINE RANDU. (SEE RANDU FOR DESCRIPTION.

DOUBLE PRECISION WNOIS, SD

CALL RANDU(ISEED, ISEED, P)
WNOIS = (P - 0.5) * 2.0 * SD

RETURN
END
SUBROUTINE RANDU

PURPOSE
COMPUTES UNIFORMLY DISTRIBUTED RANDOM REAL
NUMBERS BETWEEN 0 AND 1.0 AND RANDOM INTEGERS
BETWEEN ZERO AND 2**31. EACH ENTRY USES AS INPUT
AN INTEGER RANDOM NUMBER AND PRODUCES A NEW
INTEGER AND REAL RANDOM NUMBER.

USAGE
CALL RANDU(IY,YFL)

DESCRIPTION OF PARAMETERS
IX - FOR THE FIRST ENTRY THIS MUST CONTAIN ANY
ODD INTEGER NUMBER WITH NINE OR LESS
DIGITS. AFTER THE FIRST ENTRY, IX SHOULD BE
THE PREVIOUS VALUE OF IY COMPUTED BY THIS
SUBROUTINE.
IY - A RESULTANT INTEGER RANDOM NUMBER REQUIRED
FOR THE NEXT ENTRY TO THIS SUBROUTINE. THE
RANGE OF THIS NUMBER IS BETWEEN ZERO AND
2**31
YFL- THE RESULTANT UNIFORMLY DISTRIBUTED,
FLOATING POINT, RANDOM NUMBER IN THE RANGE
0 TO 1.0

REMARKS
THIS SUBROUTINE IS SPECIFIC TO SYSTEM/360 AND
WILL PRODUCE 2**29 TERMS BEFORE REPEATING. THE
REFERENCE BELOW DISCUSSES SEEDS (65539 HERE),
RUN PROBLEMS, AND PROBLEMS CONCERNING RANDOM
DIGITS USING THIS GENERATION SCHEME. MACLAREN
AND MARSAGLIA, JACM 12, P. 83-89, DISCUSS
CONGRELATIONAL GENERATION METHODS AND TESTS. THE
USE OF TWO GENERATORS OF THE RANDU TYPE, ONE
FILLING A TABLE AND ONE PICKING FROM THE TABLE,
IS OF BENEFIT IN SOME CASES. 65549 HAS BEEN
SUGGESTED AS A SEED WHICH HAS BETTER STATISTICAL
PROPERTIES FOR HIGH ORDER BITS OF THE GENERATED
DEVIMATE. SEEDS SHOULD BE CHOSEN IN ACCORDANCE
WITH THE DISCUSSION GIVEN IN THE REFERENCE
BELOW. ALSO, IT SHOULD BE NOTED THAT IF
FLOATING POINT RANDOM NUMBERS ARE DESIRED, AS ARE
AVAILABLE FROM RANDU, THE RANDOM CHARACTERISTICS
OF THE FLOATING POINT DEVIATES ARE MODIFIED AND
INSIST THESE DEVIATES HAVE HIGH PROBABILITY OF
HAVING A TRAILING LOW ORDER ZERO BIT IN THEIR
FRACTIONAL PART.

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
NONE

METHOD
POWER RESIDUE METHOD DISCUSSED IN IBM MANUAL
C20-8011, RANDOM NUMBER GENERATION AND TESTING

SUBROUTINE RANDU(IX, IY, YFL)
  IY=IX*65539
  IF(IY)5,6,6
  5 IY=IY+2147483647+1
  6 YFL=IY
      YFL=YFL*.4656613E-9
RETURN
END
APPENDIX B

SAMPLE PRINTED OUTPUT
(FIRST 200 SECONDS OF CASE IN FIGURE 3-9)
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APPENDIX C

ADAPTIVE TUNING LIMITS FOR BASE CASES
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**Note:** Top value is upper limit; bottom value is lower limit.
VITA

The author was born on December 21, 1955 in Baton Rouge, Louisiana to John and Catherine Balhoff. He is the seventh son in a family of eleven. Older siblings include Mike, Tom, John, Bob, Don and Bill; younger siblings include George, Margaret, Kathleen and Dan.

Elementary education was obtained at Saint Aloysius School. Secondary education was received from the Brothers of the Sacred Heart at Catholic High School.

A bachelor's degree in Chemical Engineering was received from Louisiana State University in May, 1977. Work was immediately started on a master's degree in Chemical Engineering at this same institution. This degree was obtained in May, 1979.

The author is presently employed by Shell Development Company in Houston, Texas in the process control department. The author is presently single and has no immediate plans to remedy this situation.
EXAMINATION AND THESIS REPORT

Candidate: Richard Albert Balhoff

Major Field: Chemical Engineering

Title of Thesis: Adaptive Feedforward Control of Wastewater Neutralization

Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

June 18, 1982