MODELING AND CONTROL STUDIES
OF WASTEWATER NEUTRALIZATION PROCESS

by

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ABSTRACT

In this paper, the study of the dynamics and control of a semibatch wastewater neutralization process in modeling and simulation is presented.

The wastewater neutralization process is modeled based on the reaction between a strong basic solution and a strong acidic solution in a semibatch reactor. It is assumed that the wastewater is acidic in nature. The semibatch system chosen here consists of two input streams and a mixing tank which contains an initial amount of acid solution. The initial simulation involves studying the dynamics and control of the model formulated. The objective of the control was to regulate the base flow, while keeping the acid flowrate constant, until the pH in the mixing tank stabilized at pH 7. A digital PI control algorithm was used as the controller, and the control simulation was performed in Matlab's Simulink environment.

The control studies were done to include the effect of changes in process dead time, base concentrations and base flowrates to the controllability of the semibatch system. From the simulation study, it was found that an increase in process dead time would result in process instability. While, an increase in base concentration and flowrate would result in faster neutralization time. For a given set of condition, the process dead time gave no effect to the volume of wastewater accumulated in the tank.

INTRODUCTION

Wastewater neutralization plays an important part in a wastewater treatment process. It provides the optimum environment for microorganism activity i.e. between pH 6.5 and 7.5, and the right water discharge to the public sewage as mandated by the Department of Environment of between pH 5 and 9 (Environmental Quality Act, 1974). Wastewater of pH below 4.5 and above 9 may greatly reduce the activity of the microorganisms which treat the water and may not support their life at all.

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In the neutralization process, acidic wastewater is treated with alkaline solution, while alkaline wastewater is treated with acidic solution. In either case, the wastewater is treated until it neutralized to pH 7 or any other desired pH. The process can be either operated as a continuous stirred tank (CSTR) or in batch operation. In contrast to CSTR, a semibatch operation ensures complete neutralization of wastewater present in the reactor.

The control system implemented in the neutralization process depends upon the desirable 'quality' of the treated wastewater. An on-off control system is suitable for a broad range of pH control, such as the final stage of the neutralization process, whereby the controlled range is between 5 and 9. For a narrower range of pH control, a proportional-integral (PI) control system is recommended.

Controlling the wastewater neutralization process has been known to be intrinsically difficult, due to various factors such as nonlinearity of pH system, varying process parameters (Horwitz, 1993), vessel design and process equipment used (Hoyle and McMillan, 1996), control valve characteristics (Shinskey, 2000) and type of controllers used (Shinskey, 1998).

In this paper, we intend to show the effect of varying process parameters such as reagent flowrates and concentrations and process dead time to the controllability of the wastewater neutralization using a PI controller in a semibatch reactor.

MODELING OF STRONG ACID – STRONG BASE NEUTRALIZATION PROCESS

In this study, the semibatch process model (Figure 1), consists of a mixing tank with an initial amount of acidic solution (wastewater) and of two input streams of strong acidic (wastewater) and strong basic (reagent) solutions. The aim of this process is to simultaneously neutralize the wastewater already in the mixing tank and the wastewater from the input stream by regulating the flowrate of the reagent solution F_b until the mixed solution stabilizes at pH 7. This model assumes perfect mixing and an ideal linear control valve.
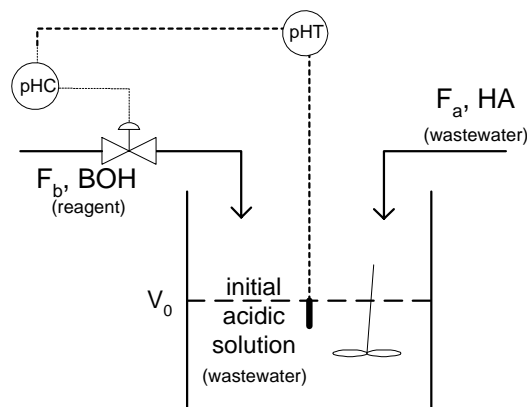

Figure 1: A semibatch pH neutralization process

The model equations for the neutralization of sulfuric acid and sodium hydroxide in a semibatch system can be written as:

The rate of volume change

$$\frac{dV}{dt} = F_a + F_b \qquad \dots\dots\dots (1)$$

Sulphate ion balance

$$\frac{d[SO_4^{2-}]}{dt} = \frac{F_a [SO_4^{2-}]_a}{V} \qquad \dots\dots\dots (2)$$

Sodium ion balance

$$\frac{d[Na^+]}{dt} = \frac{F_b [Na^+]_b}{V} \qquad \dots\dots\dots (3)$$

Electroneutrality balance

$$2 [H^+] + [Na^+] = [SO_4^{2-}] + [OH^-] \qquad \dots\dots\dots (4)$$

Water equilibrium at 25°C

$$[H^+][OH^-] = K_w = 10^{-14} \qquad \dots\dots\dots (5)$$

where the notations are given under "Nomenclature".

Equations (1) to (5) are combined together to give

$$\frac{d[H^+]}{dt} = \frac{[H^+]^2}{\{2 [H^+]^2 + K_w\}V} \left\{ F_a [SO_4^{2-}]_a - F_b [Na^+]_b \right\} \qquad \dots\dots\dots (6)$$

Equation (6) can be solved numerically for [H$^+$], while the pH of the system can be calculated as per definition:

$$pH = - \log [H^+] \qquad \dots\dots\dots (7)$$

PID CONTROL SYSTEM

The wastewater neutralization model and its associated control strategies (Figure 1) can be transformed into control block diagram as (Figure 2)
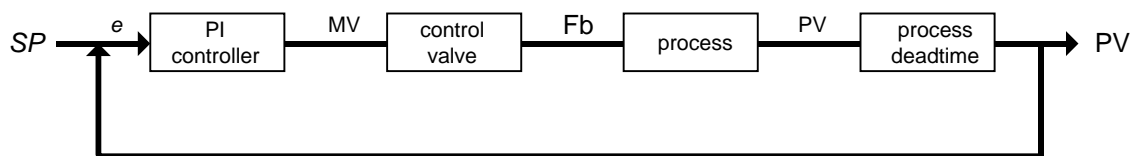

Figure 2: Control block of semibatch wastewater neutralization process.

The PI controller receives process value (PV) from process block and performs the following computation (Marlin, 1995):

$$\Delta MV = K_c \left\{ e_t - e_{t-1} + \frac{\Delta t}{I} e_t \right\} \qquad \text{.......... (8)}$$

$$MV_t = MV_{t-1} + \Delta MV_t \qquad \text{.......... (9)}$$

where MV_t represents the controller's output at current sampling time, MV_{t-1} represents the controller's output at previous sampling time, Δt represents the sampling time, e_t represents the error or the deviation from set point value at current sampling time ($SV - PV_t$), e_{t-1} represents the error at the previous sampling time, and K_c and I are the controller's tuning constants.

The computed MV_t is translated into equivalent base flowrate, F_b, by assuming that the controller's output is linearly proportional to F_b. Then, the process block uses the computed F_b to calculate the pH of the wastewater by employing (6) and (7). The process dead time block, i.e. the delay in pH signal to the controller, holds the signal for a specified amount of time (T_d). After that, the signal is sent to a comparator to calculate the error (e_t) before performing computation as in (8) and (9). This loop computation keeps repeating until the simulation is stopped.

SIMULATION FOR CONTROL OF NEUTRALIZATION PROCESS

In this simulation study, it is assumed that the wastewater is acidic in nature with a sulfuric acid concentration of $C_a = 0.00005$ M and flowrate of $F_a = 1$ L/min. An initial amount of wastewater, $V_o = 25\,\ell$, of similar concentration (0.00005 M) already present in the tank and the wastewater stream, F_a, will be neutralized simultaneously with alkaline solution of concentration C_b and flowrate F_b. The base flowrate, F_b, is set so as to simulate the maximum flow capacity through the control valve. However, during control, the F_b can be between zero flow to maximum F_b as it is being manipulated by the controller.

The wastewater characteristics and the variables selected for this study are listed in Table 1 and Table 2. The simulation approach of this study is to vary one variable at a time, while the others are set constants. Each set is run and the controller is tuned until the pH of the wastewater in the tank is about 7.

A Matlab/Simulink program has been used to solve the equations above. A sample of the Simulink program is shown in the Appendix. Table 1 and 2 show the values used in running the simulation.

Table 1: Wastewater characteristics

Wastewater	Sulfuric acid, H_2SO_4
C_a:	0.00005 M
pH_o:	4
F_a:	0.01667 ℓ/s (1 L/min)

Table 2: Variables under studies

Reagent	Sodium Hydroxide, NaOH
C_b:	0.0002, 0.0003, 0.0004, 0.0005 M
F_b:	0.025, 0.0334, 0.0417, 0.050 ℓ/s
T_d:	0, 20, 40 s

where pH_o represents the initial pH of wastewater in the tank and T_d represents the process dead time.

The objective of the simulation exercise is to control the neutralization process tightly at pH 7, without overshoot and with minimum settling time under various changes in the reagent flowrates (F_b), reagent concentrations (C_b) and process dead time (T_d). The tuning parameters (K_c and I) are initially calculated using Zieglar-Nichols (1945) method by performing a step test and fine tuned further. The various simulation studies performed are described below.

RESULT AND DISCUSSION

The results on the study of step tests and the effect of reagent flowrates, reagent concentrations and process dead time to the controllability of the neutralization process are presented below.

Step Tests

Step test was performed by making a quick change to the base flowrate, i.e. from zero flow to maximum flowrate (F_b). The result of this test provides information on the characteristics of the process, such as the neutralization time, and the initial values of the controller's setting i.e. the controller gain, K_c, and integral time, I.

The result of the step input tests performed are shown in Figure 3 and a sample of the initial values of the controller's setting, calculated using Zieglar-Nichols method, is shown in Table 3.

Table 3: Parameters for step tests of dead time variations and
the calculated K_c and I at constant C_b = 0.0002 M, F_b = 0.025 ℓ/s

Set	T_d, s	K_c	I, s
1	0	0.0973	12462
2	40	0.0962	12595
3	120	0.0942	12862

All the openloop responses shown in Figure 3 conform to the typical (Myron et. al., 1979) strong acid-strong base neutralization curves: S-shaped with inflection point at pH 7. In figure 3(a) and 3(b), increasing C_b and F_b result in faster neutralization time and wider range of steep region around pH 7.

As shown in Figure 3(c), adding process dead time to the control model, does not change the shape of the openloop response, but merely shifts the curve slightly forward. A larger shift can be observed at pH between 4.5 and 9.5 as compared to pH below 4.5 and above 9.5.
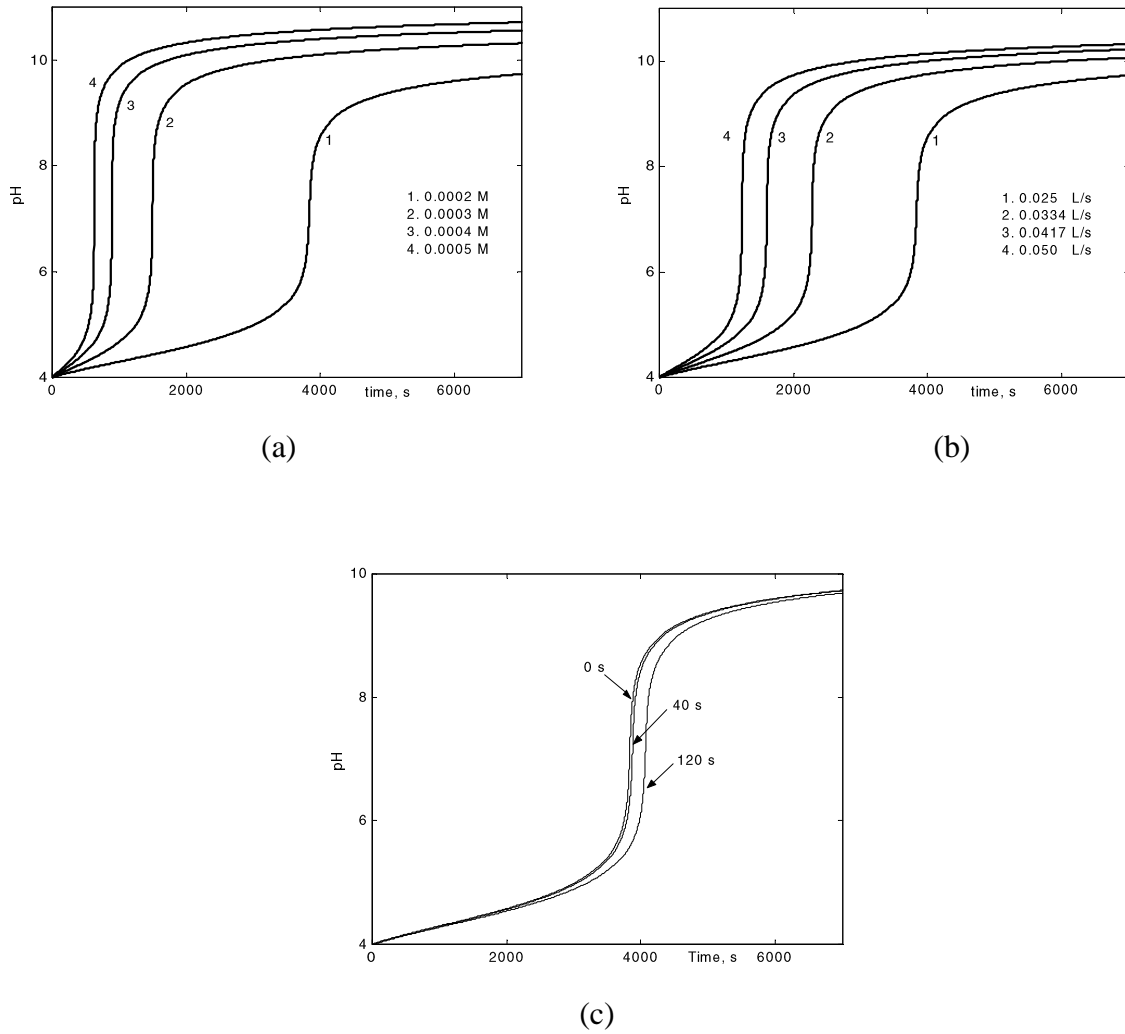
(a)

(b)

(c)

Figure 3: Neutralization curves of H_2SO_4-NaOH in semibatch reactor. (a) Step tests with C_b variation. (b) Step tests with F_b variation. (c) Step tests with T_d variation.

Effect of base concentration to the controllability at neutralization pH

In this study, the dead time was held constant at 0 s, F_b was regulated between 0 and 0.025 ℓ/s and C_b was set at 0.0002 to 0.0005 M in steps of 0.0001 M. Table 4 shows the C_b variations and the K_c and I used in the simulation, while Figure 4 shows the result of the simulation.

Table 4: Values of C_b and K_c used in the simulation. I was set at 3 s.

Set	C_b, M	K_c
1	0.0002	1
2	0.0003	0.4
3	0.0004	0.2
4	0.0005	0.12

From Figure 4(a), the control of the neutralization showed a near perfect control once pH 7 is achieved. In Figure 4(b), the regulated F_b started at 0.025 ℓ/s, but upon passing the neutralization pH, F_b dropped sharply to the value that stoichiometrically neutralized the wastewater stream F_a. An increase in C_b results in faster neutralization time and lesser F_b used after the neutralization time. Consequently, the overall volume accumulated which dependent on F_b, decreases with higher C_b. Figure 4(c) shows the overall volume accumulated with increasing C_b.
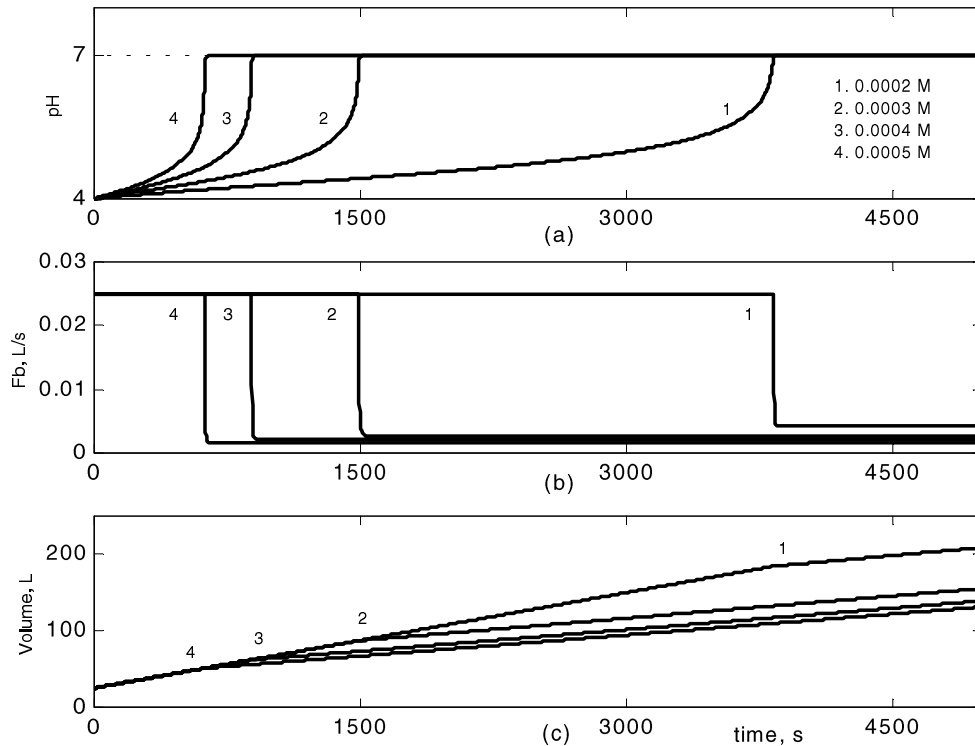

Figure 4: Effect of C_b to the controllability at the neutralization pH. (a) pH response. (b) manipulated variable F_b. (c) Overall volume accumulated

Effect of base flowrates to controllability at neutralization pH

Here, the variable C_b and T_d were held constant at 0.0002 M and 0 s, respectively. The base flowrate was regulated between 0 and F_b, which was set at 0.025 to 0.05 ℓ/s in step of 0.0053 ℓ/s. Table 5 shows the variation of F_b and the values of K_c and I used in the simulation. Figure 6 shows the result of the simulation.

Table 5: The values of F_b and K_c used in the simulation. I was set at 3 s.

Set	F_b	K_c
1	0.025	1
2	0.033	0.9
3	0.042	0.8
4	0.050	0.7

The effect of F_b to the controllability at neutralization pH is very much similar to the effect of C_b as elaborated earlier.

As shown in Figure 5(a), the controllability at the neutralization pH shows a near perfect control, and an increase in F_b results in faster neutralization time. In Figure 5(b), the regulated F_b started at the maximum value F_b but upon passing the neutralization pH, F_b dropped sharply to a value that stoichiometrically neutralized the wastewater stream F_a. The overall volume accumulated in the tank decreases with higher F_b.
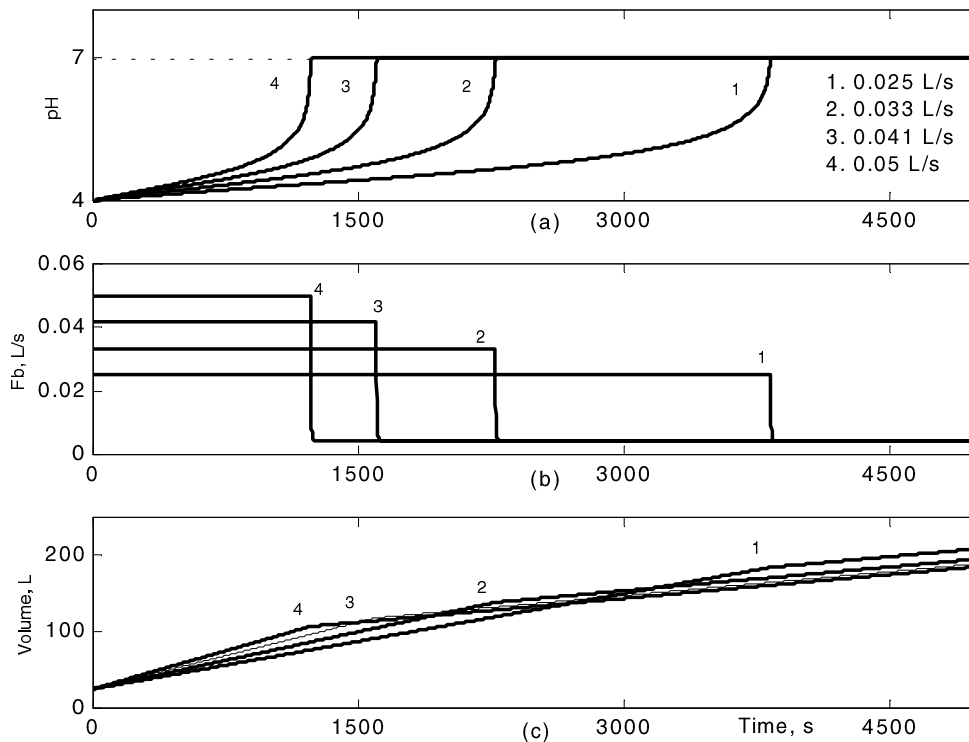

Figure 5: Effect of F_b to the controllability at the neutralization pH. (a) pH responses. (b) manipulated variable F_b. (c) Overall volume accumulated.

Effect of dead time to controllability at neutralization pH

The variables C_b was held constant at 0.0002 M. The F_b was regulated between 0 and 0.025 ℓ/s. The dead time (T_d) under study was set at 0, 40 and 120 s. Table 6 shows the variation of T_d and the K_c and I used in the simulation, while Figure 6 shows the result of the simulation.

Table 6: Values of T_d, K_c and I used in the simulation.

Set	dt, s	K_c	I, s
1	0	1	3
2	40	0.01	120
3	120	0.006	240

As shown in Figure 6(a), an increase in dead time makes the controllability harder and the settling time becomes longer. However, the overall volume accumulated in the tank, Fig. 6(c), is approximately the same for all cases. The controller gain, K_c, decreases and integral time, I, increases with increasing dead time.
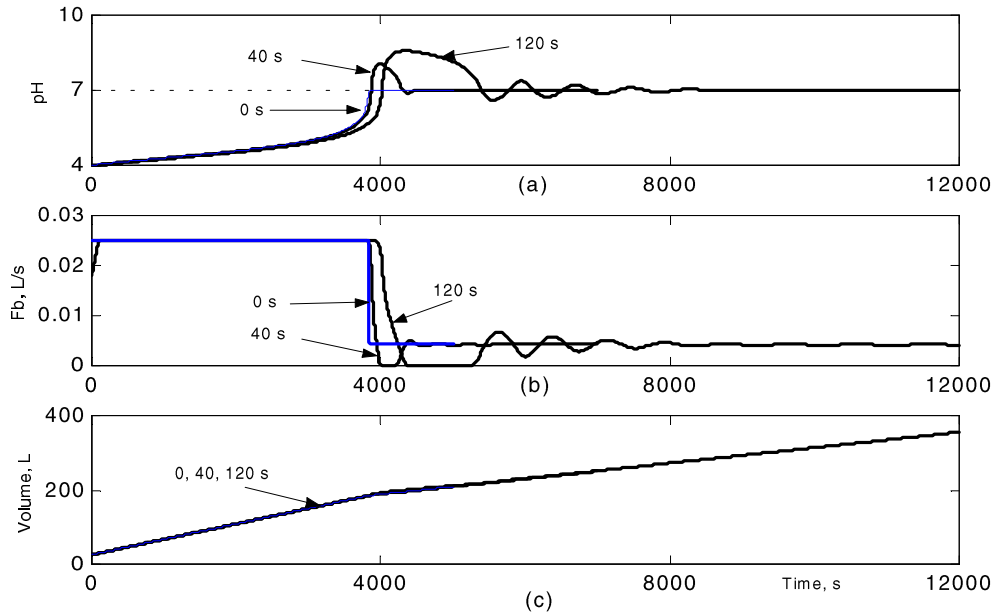

Figure 6: Effect of T_d to the controllability at the neutralization pH. (a) pH responses. (b) Manipulated variable F_b. (c) Overall volume accumulated.

CONCLUSION

It has been shown that a perfect control of semibatch wastewater neutralization is achieved in the study of the effect of base concentrations and base flowrates with no dead time. It has been shown also that the present of dead time complicates the controllability at the neutralization pH.

Further study using advanced control strategies is recommended in improving the controllability of the wastewater neutralization with long dead time present in the system.

Acknowledgement

NOMENCLATURE

C_a = concentration of the acid solution, mol/liter
C_b = concentration of the basic solution, mol/liter
F_a = flowrate of acid solution, liter/s
F_b = flowrate of basic solution, liter/s
K_c = controller gain
I = integral time, s

D   = derivative time, s

e   = error or SP – PV

e_t = error at current sampling time

e_{t-1} = error at previous sampling time

SP = setpoint, pH

pHC = pH controller

pHT = pH transmitter

PV = process value, pH

V_o = initial volume of the solution at time = 0

V   = volume of the solution after time > 0

T_d = process dead time, s

T_s = settling time, s, or time taken by the process to stabilize at SP

Δt = sampling time, s

$[H^+]$ = hydrogen ion concentration in mixing tank after time > 0, M

$[H^+]_o$ = initial hydrogen ion concentration in mixing tank, M

$[SO_4^{2-}]$ = sulphate ion concentration in the tank, M

$[SO_4^{2-}]_a$ = sulphate ion concentration in stream a, M

$[Na^+]$ = sodium ion concentration in the tank, M

$[Na^+]_b$ = sodium ion concentration in stream b, M

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APPENDIX

Matlab/Simulink block program used for the simulation of semibatch wastewater neutralization