

## EFFECT OF VALVE CHARACTERISTICS TO THE CONTROLLABILITY OF pH IN A CONTINUOUS STIRRED TANK REACTOR

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### Abstract

In this paper, simulation work on the effect of equal percentage and linear control valves to the controllability of pH in a continuous stirred tank reactor (CSTR) using a PI controller is presented. The simulation result showed that at initial start up, in neutralizing the acidic solution in the reactor from pH 4 to a new set point, an equal percentage control valve performed better than a linear control. However, after stabilizing to a new set point, the linear control valve out performed the equal percentage control valve. These effects were attributed to the different rate of change in manipulated variable per change in controller's output at initial start up and at the new set point in both equal percentage and linear control valves. Details of the simulation work involved is presented in this paper.

*Keywords:* Control valves, PID control, pH control, valve characteristics.

### 1.0 INTRODUCTION

Control valves are the most found final control elements used in chemical process industries to regulate flowrates. These variation in flowrates will affect any controlled variables that is related to it such as temperature, level, pressure, pH and flow itself. The rate of change in flow for a given input signal to the control valve depends on valve's flow characteristics i.e. linear, equal percentage or quick opening.

The linear valve provides a flowrate directly proportional to the stem's travel and it is used when the pressure accross the control valve is approximately constant such as in certain cases of level and flow loops. An equal percentage valve produces an equal percentage change in flowrate for every equal increment of stem's travel. It is often used when the pressure drop accross the control valve is not constant. This occurs when there are other equipments in the system that act as fixed resistances such as heat exchanger or vessel systems [1]. Unlike linear and equal percentage valves, the quick opening valve permits 70% of its flow capacity for the first 40% of valve opening. For this reason, quick opening valve is mostly used in over-pressure relief system [2,3]. The rule of thumbs and guideline in selecting control valve's flow characteristics based on pressure drop has been summarized by Harrold and Liptak [4,5].

The complication of valve characteristics to the controllability of neutralization process has been noted by Shinsky and Gary [6,7,8]. Attributing to variation in pressure drop accross control valve and the nonlinear response of pH, they have suggested a "software characterizer" be placed between the setpoint and pH measurement blocks. It is a mathematical function that will linearize the logarithmic response of pH. Eventually, the flowrate variation becomes linear with controller's output.

This paper intends to compare the behavior of pH of a neutralization process in a CSTR using two different valve characteristics i.e. linear and equal percentage. In this work, the flowrate varies according to the valve characteristics. The performance of each valve characteristic is tested to handle load disturbances and changes in set points.

## 2.0 MODELING AND CONTROL OF A CSTR NEUTRALIZATION SYSTEM

In this study, a continuous stirred tank reactor (CSTR) process model, Fig. 1, consists of a mixing tank with an initial amount of acid solution and two input streams of strong acid and strong base solutions. The aim of this process is to simultaneously neutralize the acid solution already in the mixing tank and the acid solution from the input stream,  $F_a$ , by regulating the flowrate,  $F_b$ , of the base solution until the mixed solution stabilizes at pH 7. This model assumes perfect mixing.

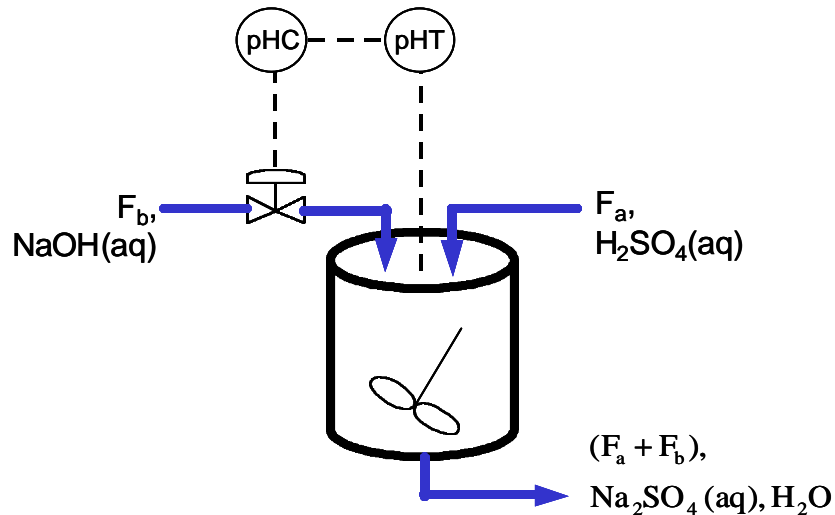


Figure 1: pH neutralization in a CSTR and its associated control scheme.

The following paragraph will briefly explain the modeling and control of this CSTR neutralization strategy.

### 2.1 Modeling a CSTR neutralization process

The model equations for the neutralization of sulfuric acid (strong acid) and sodium hydroxide (strong base) in a CSTR system can be written as:

Sulphate ion balance

$$\frac{V d[SO_4^{2-}]}{dt} = F_a [SO_4^{2-}]_a - (F_a + F_b)[SO_4^{2-}] \quad \dots\dots\dots (1)$$

Sodium ion balance

$$\frac{V d[Na^+]}{dt} = F_b [Na^+]_b - (F_a + F_b)[Na^+] \quad \dots\dots\dots (2)$$

Electroneutrality balance

$$2 [H^+] + [Na^+] = [SO_4^{2-}] + [OH^-] \quad \dots\dots\dots (3)$$

Water equilibrium at 25°C

$$[H^+][OH^-] = K_w = 10^{-14} \quad \dots\dots\dots (4)$$

where,  $V$  is the CSTR volume ( $\ell$ ),  $F_a$  is the flowrate of the acidic solution ( $\ell/s$ ),  $F_b$  is the flowrate of the basic solution ( $\ell/s$ ),  $[H^+]$  is the concentration of hydrogen ion (M),  $[OH^-]$  is the concentration of hydroxyl ion in CSTR (M),  $[Na^+]$  is the concentration of sodium ion in CSTR (M),  $[Na^+]_b$  is the concentration of sodium ion in stream  $F_b$  (M),  $[SO_4^{2-}]$  is the concentration of sulphate ion in CSTR (M),  $[SO_4^{2-}]_a$  is the concentration of sulphate ion in stream  $F_a$  (M); and  $K_w$  is the water dissociation constant.

Equations (1) to (4) are combined together to give

$$\frac{d[H^+]}{dt} = \frac{[H^+]\{F_a [SO_4^{2-}]_a [H^+] - F_b [Na^+]_b [H^+] - (F_a + F_b)(2[H^+]^2 - K_w)\}}{\{2[H^+]^2 + K_w\}V} \dots\dots\dots (5)$$

Equation (5) is then solved numerically for  $[H^+]$ . Accordingly, the pH in the neutralization tank can be computed as

$$pH = - \log [H^+] \dots\dots\dots (6)$$

### 2.2 Controller

A discretized PI controller [9] has been chosen as the controller in this work as shown below.

$$\Delta MV = K_c \left\{ e_t - e_{t-1} + \frac{\Delta t}{I} e_t \right\} \dots\dots\dots (7)$$

$$MV_t = MV_{t-1} + \Delta MV_t \dots\dots\dots (8)$$

where  $MV_t$  represents the controller's output at the current sampling time,  $MV_{t-1}$  represents the controller's output at the previous sampling time,  $\Delta t$  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.

### 2.3 Control valve characteristics

Control valve characteristic is defined as the relationship between valve travel (stem position) and valve's flow capacity under constant pressure drop conditions [2]. There are two main valve characteristics used for control purposes: namely, linear and equal percentage. A linear valve has direct relationship between the valve travel and the flow capacity. But, in equal percentage valve, the flow capacity changed by percentage of every increment in valve travel. In this simulation study, the relationship that has been developed by Shinsky [8] in approximating the characteristics of linear and equal percentage valves will be used. Equation (9) shows the relationship used by Shinsky, while Figure 3 shows the graphical representation of Eq. (9).

$$y = \frac{x}{L + (1-L)x} \dots\dots\dots (9)$$

where,  $y$  is the control valve's output,  $x$  is the control valve input, and  $L$  is equal to 1 for linear and 5 for equal percentage.

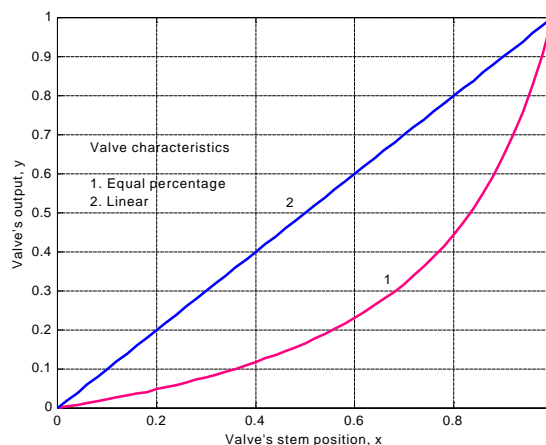


Figure 3: Characteristics of linear and equal percentage valve.

## 2.4 Control simulation approach

The strong acid – strong base neutralization model and its associated control scheme, Fig.1, can be transformed into control block diagram as in Fig. 2.

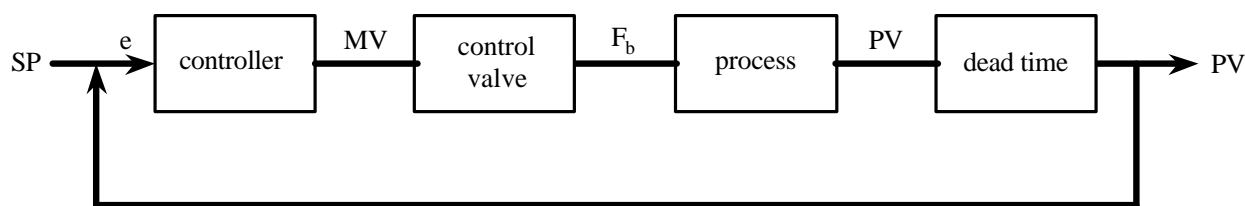


Figure 2: Control blocks of pH control in a CSTR.

As shown in Fig. 2, a PI controller receives process measurement value (PV) and compares it with the set point (SP). The controller calculates the error (i.e.  $SV-PV$ ) and performs computation as in Eq. (7). Then, the controller outputs an appropriate signal (MV) based on Eq. (8) to determine the valve's stem position. In this simulation work, Eq. (9) is used to simulate a linear or an equal percentage valve. Output from the control valve is the base flowrate ( $F_b$ ), which in turn is used in Eq. (5) and (6) to calculate the next process value ( $PV_{t+1}$ ). Then, the process value ( $PV_{t+1}$ ) is kept for the duration of process deadtime ( $T_d$ ) before being sent to the controller for the next computation.

## 2.4 Simulation parameters

The simulation parameters used in this study is shown in Table 1. These parameters were all used in the simulation work.

Table 1: Simulation parameters

Parameters	Values
Reactor volume, $V$ ( $\ell$ )	25
Initial pH in reactor, pH	4
Flowrate of acidic solution, $F_a$ ( $\ell/s$ )	0.033
Flowrate of basic solution, $F_b$ ( $\ell/s$ )	0 to 0.05
Concentration of acidic solution, $[H_2SO_4]$ (M)	0.00005
Concentration of basic solution, $[NaOH]$ (M)	0.0002
Process deadtime, $T_d$ (s)	40
Tuning constant, $K_c$	0.001
Tuning constant, $I$	120

## 3.0 RESULT and DISCUSSION

Result of the simulation work is shown in Fig. 4 and 5 and summarized in term of settling time and IAE as in Table 2 and 3. Figure 4 shows the responses toward load disturbances, while Fig. 5 shows the responses toward changes in set points.

Table 2: Comparison between equal percentage and linear valves under load disturbances

Valves	Change in $Ca$ (pH)	$T_s$ (s)	IAE	Change in $F_a$ (L/s)	$T_s$ (s)	IAE
Eq. %	4 to 3 to 5 to 4	4807	6103	0.033 to 0.066 ..	3384	2430
Linear	4 to 3 to 5 to 4	3814	5559	.. to 0.016 to 0.033	2343	2688

As shown in Fig. 4(a), at initial start up, an equal percentage valve took 5057 s to stabilize the process to pH 7 compared to a linear valve which took 4645 s. In term of IAE, the equal percentage valve has lower IAE than the linear valve as shown in Table 3. When the process has stabilized at the set point, pH 7, a load disturbance (i.e. variation in acid concentrations) is made at  $t = 7000$  s. Both of the control valves responded immediately to the changes in pH and stabilized the process back to pH 7. The linear valve stabilized the process in 3814 s with IAE of 5558 compared to the equal percentage valve in 4807 s with IAE of 6103. The next load disturbance (i.e. variation in acid flowrates) is made at  $t = 14000$  s. The linear valve stabilized the process in 2343 s compared to the equal percentage valve in 3384 s. However, the equal percentage valve has slightly lower IAE (2430) than the linear valve (2688). The final stem position at steady state is 16.6%

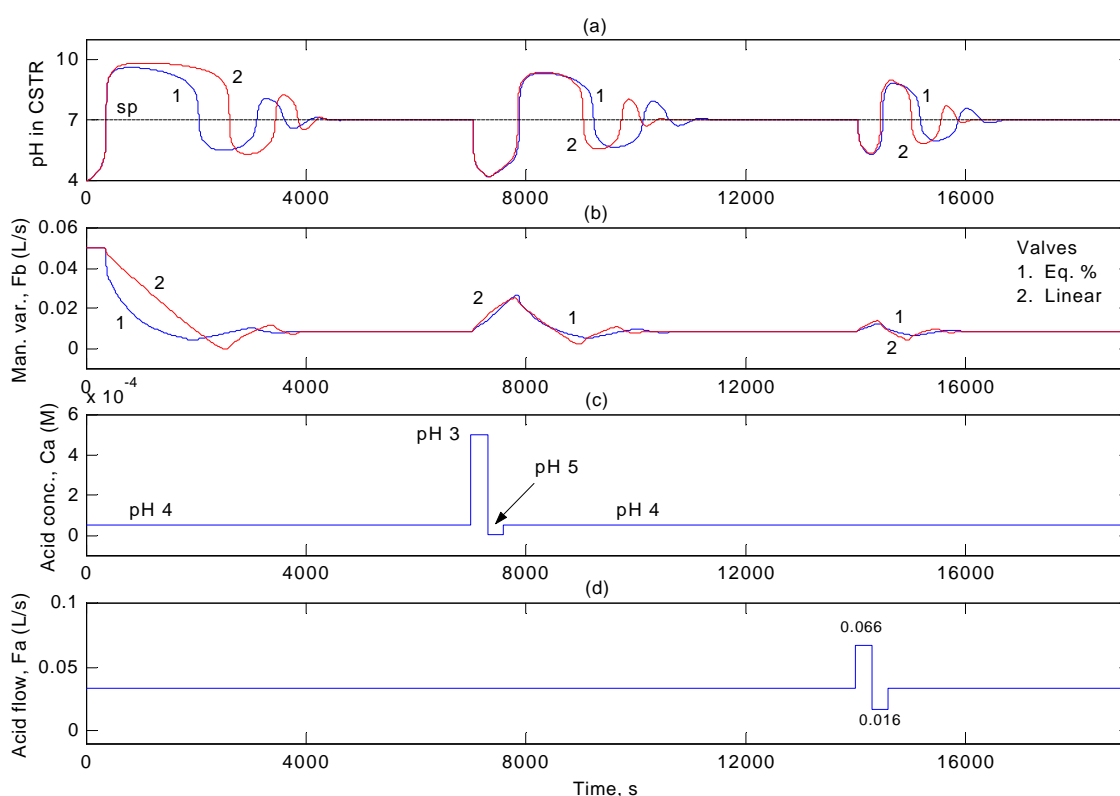


Figure 4: pH responses at initial start up and toward load disturbances.

The performance of both control valve was also tested to handle changes in set points as shown in Fig. 5. At initial start up, both of the control valve stabilized the process to the set point, pH 8, relatively close to each other (equal percentage,  $T_s = 6366$  s; linear,  $T_s = 6350$  s). However, the equal percentage valve has significantly lower IAE (5343) than the linear valve (7337). At  $t = 8000$  s, the set point was changed to pH 6, while at  $t = 12000$  s, the set point was changed to pH 7. In both of the changes in set points, the linear valve out-performed the equal percentage valve in term of settling time and IAE as shown in Table 3. The final stem positions depended on the set points as shown in Table 3.

Table 3: Comparison between equal percentage and linear valves under set point change

Set point change	Ts (s)		IAE		Final valve's stem position
	Eq. %	Linear	Eq. %	Linear	
4 to 7	5057	4645	6601	8374	16.6%
4 to 8	6366	6350	5343	7337	17.1%
8 to 6	4578	4111	592	453	15.7%
6 to 7	2900	2527	453	309	16.6%

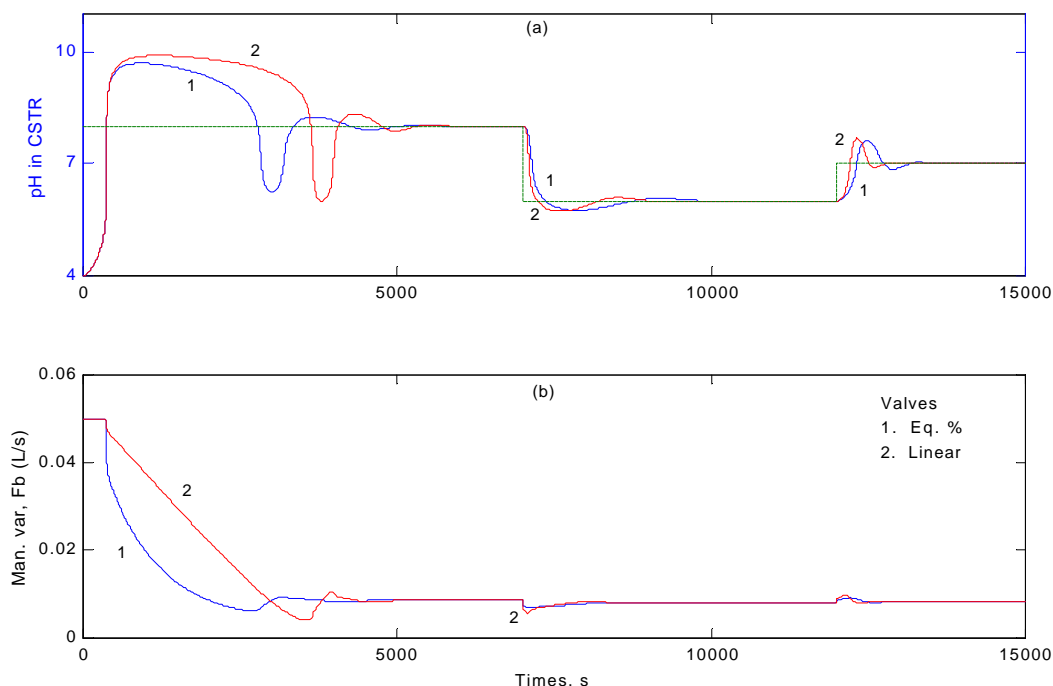


Figure 5: pH responses toward changes in set points.

From the above results, the equal percentage valve is suitable than the linear valve in handling the initial start up process. The reason is that in equal percentage valve, starting at 100% valve's stem position, the valve characteristic values drop faster than of linear valve as shown in Fig. 3. As the result, the overshoot and IAE can be reduced. This drastic reduction in flowrate can be observed in Fig. 4(b) and 5(b). On the other side, flowrate of the linear valve, dropped linearly with the valve characteristics.

Upon stabilizing at the set point, the stem position is between 15 to 17% in both linear and equal percentage valves. Within this range, the equal percentage valve has a very low characteristic value than the linear valve as shown in Fig. 3. Consequently, upon load disturbances (i.e. variations in acid flowrates and concentrations) and changes in set points, an equal percentage valve will response slower than a linear valve. In turn, the settling time became longer.

#### 4.0 CONCLUSION

The effect of linear and equal percentage valves to the controllability of pH in a CSTR system has been shown. It has been shown that an equal percentage valve is more suitable at initial start up process, while a linear valve is more suitable in handling load disturbances and changes in set points. It may not be probable to install two types of control valve in a control loop, but a linear valve plus a mathematical function to emulate equal percentage valve can be used.

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## **6.0 REFERENCES**

1. Shinskey, F.G., "The Three Faces of Control Valves", Control Engineering, July 2000, pp 83-86
2. Harrold, D., "Control Valves: Match Size with Application", Control Engineering, Sept. 1999, pp 93-98
3. Schaufbuch, P., "Fundamentals of Flow Characterization", Fisher-Rosemount, Technical Monograph No. 29
4. Liptak, B.G. & Matley, J. (Ed), "Practical Process Instrumentation and Control: Control Valves in Optimized Systems", McGraw-Hill, 1986, pp 245-252
5. Harrold, D., "Control Valve Characteristic Guidelines", Control Engineering Online, <http://www.manufacturing.net/ctl/index.asp?layout=articleWebzine&articleID=CA188508>
6. Shinskey, F.G. & Gerry, J., "Neutralize pH Control System Instabilities", <http://www.expertune.com/articles/neutralizepH/neutralizeph.html>
7. Shinskey, F.G., "Characterizers for Control Loops", <http://www.expertune.com/artcharact.html>
8. Marlin, T.E., "Process Control: Designing Processes and Control Systems for Dynamic Performance, McGraw-Hill, 1995, pp 386-387
9. Luyben, W.L., "Process Modeling, Simulation and Control for Chemical Engineers", Mc-Graw-Hill, 2nd. Ed., 1990, pp 220-221