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Dynamic and Control of a pH-CSTR

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Abstract: This research aims to study by numerical simulation the dynamic and the control of a pH-CSTR (Continuous Stirred Tank Reactor) process. The main characteristic of this important system is that it used to neutralize an acidic inlet liquid stream so as at the exit of the continuous stirred tank reactor (CSTR) the liquid stream has a neutral pH (pH =7). The study of the pH-CSTR is carried out in order to evidence the dynamic and the influence of disturbances on the regulation of the pH inside the reactor. The controlled variable is the pH inside and at the effluent of the reactor, and the manipulative variable is the alkali (NaOH) liquid stream. The obtained results show that the PID controller can regulate the pH in the reactor at the desired set-point value despite the occurrence of strong disturbances related to the acidic composition and flow rate of the inlet liquid stream.

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1. Introduction

This research focuses on the study of pH-CSTR (Continuous Stirred Tank Reactor) because it is very used in the chemical industries and waste water processing stations. [1]. The ph-CSTR is used to neutralize an acidic inlet liquid stream by mixing it with an alkali liquid stream in order to obtain a neutral liquid stream having a pH equal or close to 7. The incoming acidic liquid stream feeding the reactor can be a liquid process or a liquid resulting of a waste water processing unit [1–3]. Indeed, a liquid stream must be processing in order to have a neutral pH before being released in the environment. These considerations motivate the need of investigating the dynamic and control of a pH CSTR system. For this purpose, the dynamic mathematical model of a pH-CSTR was set and solved using the data related to a nominal operating point. Afterwards, the performance of a PID controller was assessed in regulation and tracking mode of the pH inside the reactor.

2. The pH CSTR Unit

A flowsheet of pH-CSTR unit is presented in Figure 1 [1]. This unit consists mainly of a continuous stirred tank reactor. The feed entering the reactor is an acidic liquid. The controller manipulates an alkali liquid stream flowrate by mixing it with the inlet liquid inside the reactor. At the exit of the reactor, the effluent liquid must have a neutral pH. Table 1 gives additional parameter values related to the studied process.

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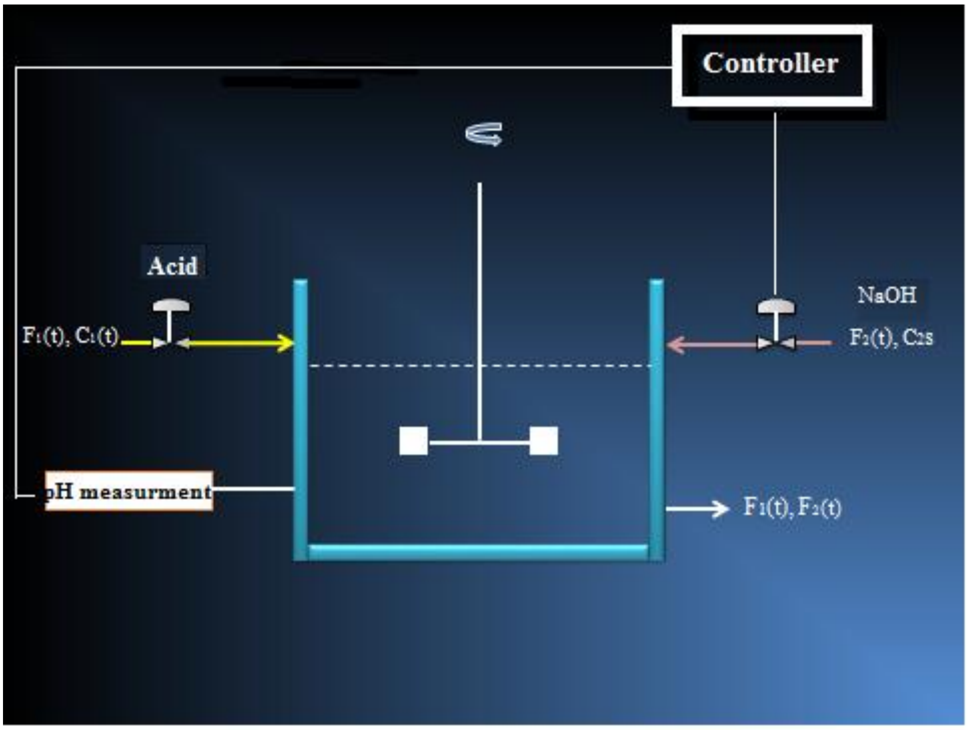

Figure 1. Flowsheet of the pH-CSTR unit [1].

Table 1. Parameters values for the ph-CSTR [1].

Parameter	Signification	Value
V	reactor volume	1000 litres
F_1	acid	81 litres/min
F_2	Alacal flowrate	515 litres/min
C_1	acid concentration	0.32 mole/litre
C_{2s}	inlet alkali concentration	0.05 mole/litre
Ka	acidity constant	10^{-5}
Kw	water ionic constant	10^{-7}

3. Model Assumptions

The main model assumptions are listed below:

- neutralization of weak acid (acetic acid) with strong alkali (NaOH) ;
- isothermal operation (constant temperature in the reactor);
- perfect mixing in the reactor;
- the dynamics of the pH sensor and valve are neglected;
- any delay time or dead time is neglected in the process;
- the concentration C_{2s} is supposed constant;
- F_2 is considered as the manipulative variable;
- disturbances are related to the acid flowrate F_1 or the acid concentration C_1.

4. Dynamic Mathematical Model and Method of Resolution

The dynamic mathematical model can be either used for studying the parametric sensivity of a process [4] or for control purpose [5]. The pH-CSTR dynamic model process is presented as follows.

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$$HAC \rightleftharpoons H^+ + AC^- \tag{1}$$

$$K_a = [H^+]\,[AC^-] / [HAC]$$

$$NaOH \rightarrow Na^+ + OH^-$$

$$HAC + NaOH \rightarrow (AC^-, Na^+) + H_2O \tag{2}$$

$$H_2O \rightleftharpoons H^+ + OH^- \qquad K_w = [OH^-]\,[H^+]$$

Molar balance for the acid

$$\xi(t) = [AC^-] + [HAC] \tag{3}$$

$$F_1(t) \,.\, C_1(t) = (F_1(t) + F_2(t)) \,.\, \xi(t) + V \,.\, d\xi(t) / dt$$

$$\Rightarrow d\,\xi(t) / dt = [(F_1(t) \,.\, C_1(t)) / V] - [((F_1(t) + F_2(t)) / V) \,.\, \xi(t) \tag{4}$$

$$\xi(t) = y_1(t)$$

Molar balance for the alkali

$$\zeta(t) = [Na^+] \tag{5}$$

$$F_2(t) \,.\, C_{2s} = (F_1(t) + F_2(t)) \,.\, \zeta(t) + V \,.\, d\,\zeta(t) / dt$$

$$\Rightarrow d\,\zeta(t) / dt = [(F_2(t) \,.\, C_{2S}) / V] - [((F_1(t) + F_2(t)) / V) \,.\, \zeta(t) \tag{6}$$

$$\zeta(t) = y_2(t)$$

Equation of the electric neutrality

$$[H^+] + [Na^+] = [OH^-] + [AC^-]$$

$$[H^+] + \zeta(t) = K_w / [H^+] + K_a \,.\, [HAC] / [H^+] \tag{7}$$

equation (1), gives :

$$[AC^-] = K_a \,.\, [HAC] / [H^+] \tag{7a}$$

the substitution of equation (7a) in equation (3), lead to :

$$\xi(t) = K_a\,[HAC] / [H^+] + [HAC] = [HAC] \,.\, [(K_a / [H^+]) + 1] \tag{3a}$$

the equation (3a) gives :

$$[HAC] = \xi(t) \,.\, [H^+] / (K_a + [H^+]) \tag{3b}$$

Finally, the substitution of equation (3b) in equation (3a) lead to a third order algebraic equation relatively to $[H^+]$:

$$[H^+]^3 + (K_a + \zeta(t)) \,.\, [H^+]^2 + (K_a \,.\, \zeta(t) - K_w - K_a \,.\, \xi(t)) \,.\, [H^+] - K_a \,.\, K_w = 0 \tag{8}$$

The resolution of the dynamic model can be resumed by the following steps:

1. Compute $\xi(t)$, from the following equation, by using Euler method

$$d\,\xi(t) / dt = [(F_1(t) \,.\, C_1(t)) / V] - [((F_1(t) + F_2(t)) / V) \,.\, \xi(t)$$

2. Compute $\zeta\,(t)$, from the following, equation by using Euler method

$$d\,\zeta\,(t)\,/\,dt = [(F_2(t)\,.\,C_{2S})\,/\,V] - [((F_1\,(t) + F_2\,(t))\,/\,V)\,.\,\zeta\,(t)$$

3. Compute the concentration $[H^+]$, from the following equation, by using Newton-Raphson method:

$$[H^+]^3 + (K_a + \zeta\,(t))\,.\,[H^+]^2 + (K_a\,.\,\zeta\,(t) - K_w - K_a\,.\,\xi\,(t))\,.\,[H^+] - K_a\,.\,K_w = 0$$

4. Compute pH from the following equation:

$$pH = -\log\,[H+]$$

5. Results and Discussion

5.1. Study of Dynamic of the Process in Open Loop Mode (Without Control)

Figure 2 show the variation of the pH in case of an occurrence of a disturbance related to C1, injected at 1 minute, equal to +10 %, during 10 seconds.. It can be seen that the system is very sensitive to the concentration of the incoming acidic flowrate; this effect can be explained by the fact that the increase of the acid concentration induces a decrease of the pH because the mixture inside the reactor becomes more acidic. Furthermore, it can be seen from Figure 2 that after the disturbance has disappeared, the pH return to its initial value. That last fact means that the system is naturally stable and it possesses a certain tendency to auto-regulate or auto-control itself.

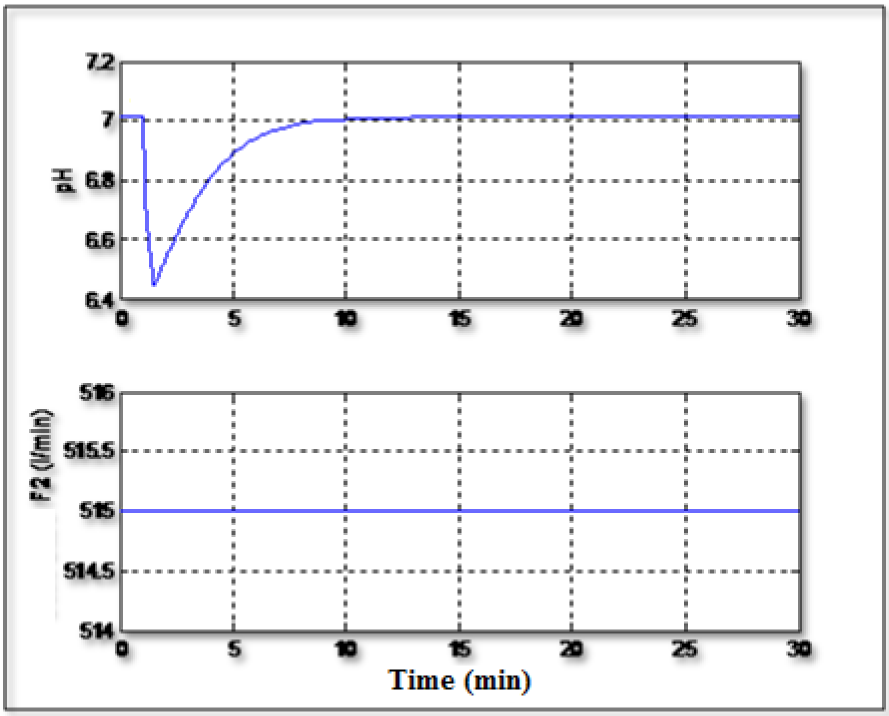

Figure 2. Variation of the pH without control in case of an occurrence of a disturbance related to C_1, injected at 1 minute, equal to +10%, during 10 seconds.

Figure 3 show the variation of the pH in case of an occurrence of a step variation related to F2, injected at 10 minute, equal to +10 %.. It can be seen that the system hasn't a dead time and he has a sigmoid response, which denotes that it is a first order process. So, from data obtained in Figure 3, the transfer function of the process was: $H(p) = K/\,(1+\tau.p) = 0.087/(1+0.06p)$

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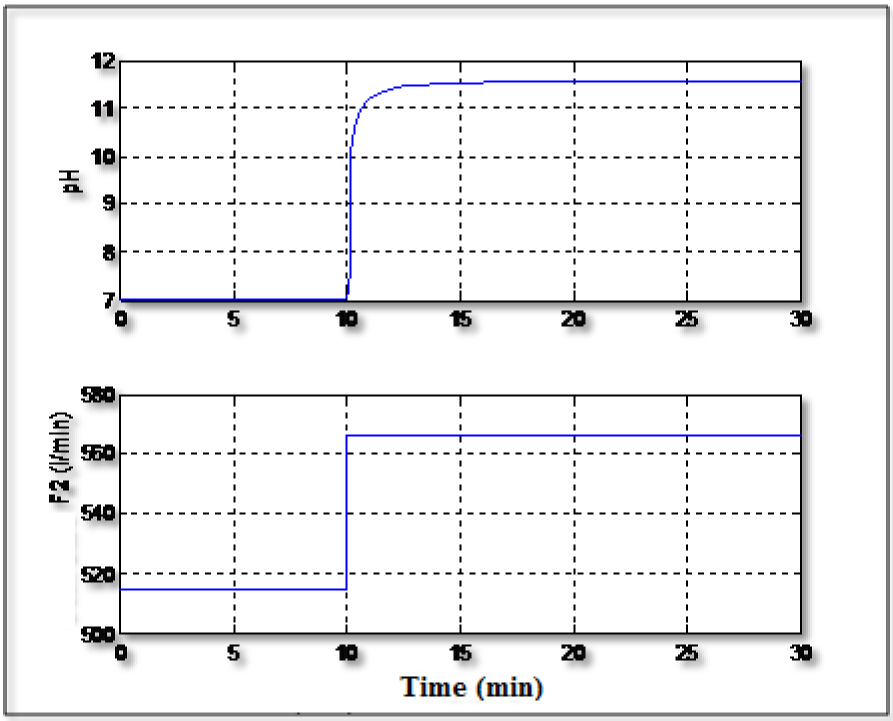

Figure 3. Variation of the pH without control in case of an occurrence of a step variation related to F_2, injected at 10 minute, equal to +10%.

The parameters of the controller were determined according to Ziegler-Nichols method by occurring continuous oscillations related to the pH in order to determine the period of the oscillations Tz . From Figure 4, the value of Tz was found to be equal to 0.2 min. Therefore, the parameters of the PID controller were found as follows : kc = 232; τ_I = 0.1 min; τ_D = 0.025 min.

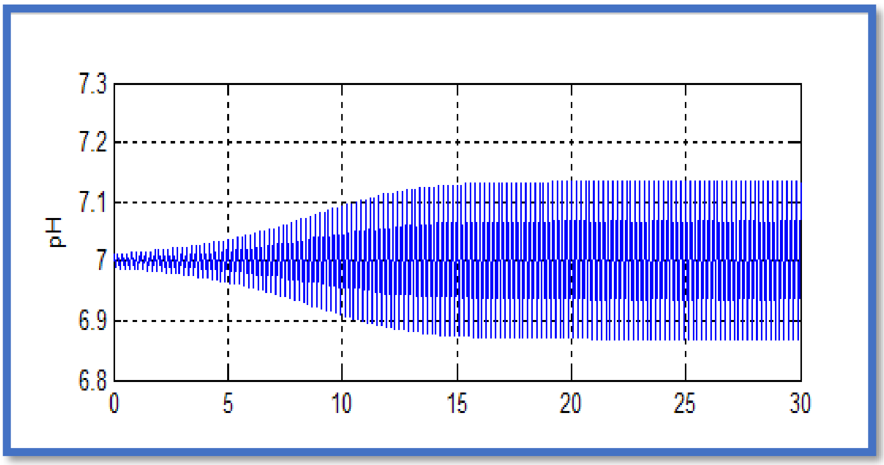

Figure 4. Continuous oscillations related to the pH.

5.1. Study of Dynamic of the Process in Closed Loop Mode (With Control)

Figure 5 shows the regulation of the pH to the setpoint value (pH =7) without occurrence of any disturbances. It can be seen from this figure that the controller can control the pH rapidly and with a good precision. The control signal (F_2) varies regularly and doesn't show excessive and dangerous peaks.

Figure 6 shows the regulation of the pH to the setpoint value (pH =7) with occurrence of a disturbance related to the concentration C_1. It can be seen that the controller can handle the disturbance and it can regulate the pH to its serpoint value and the signal control varies regularly without excessive activity.

Figure 7 shows the control of the pH in tracking mode where the value of the setpoint changes from 7 to 6. It can be seen that the controller can handle easily the variation of the setpoint value and the signal control varies regularly without excessive variations.

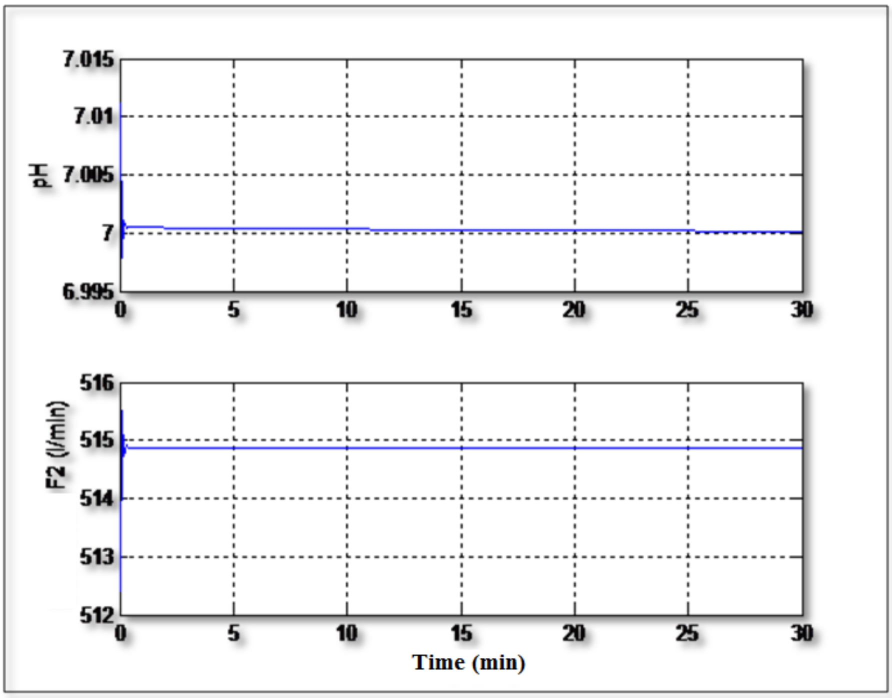

Figure 5. Regulation of the pH to the setpoint value (pH =7) without occurrence of disturbances.

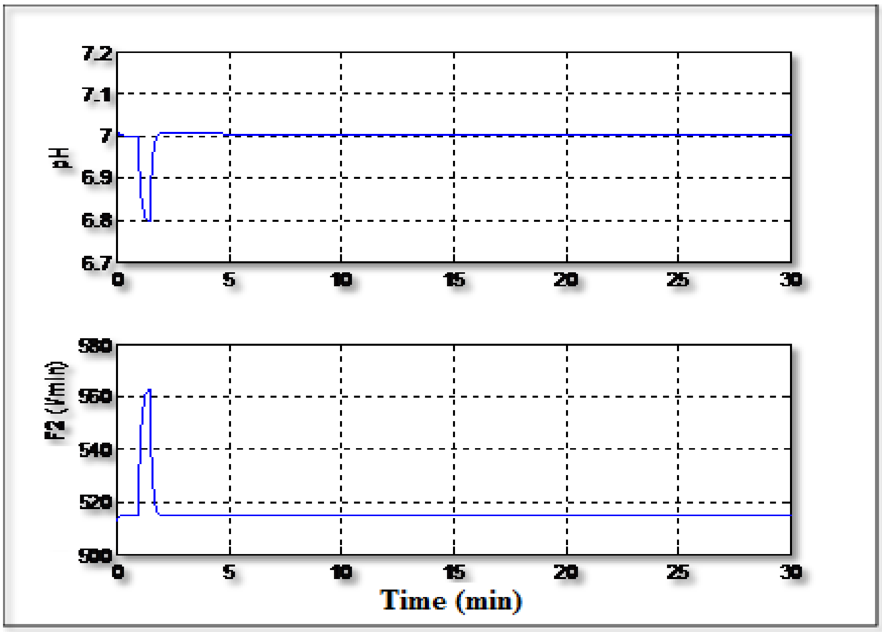

Figure 6. Regulation of the pH to the setpoint value (pH =7) with occurrence of a disturbance related to concentration C_1 equal to + 10 %, injected at t = 1 min, during 30 s.

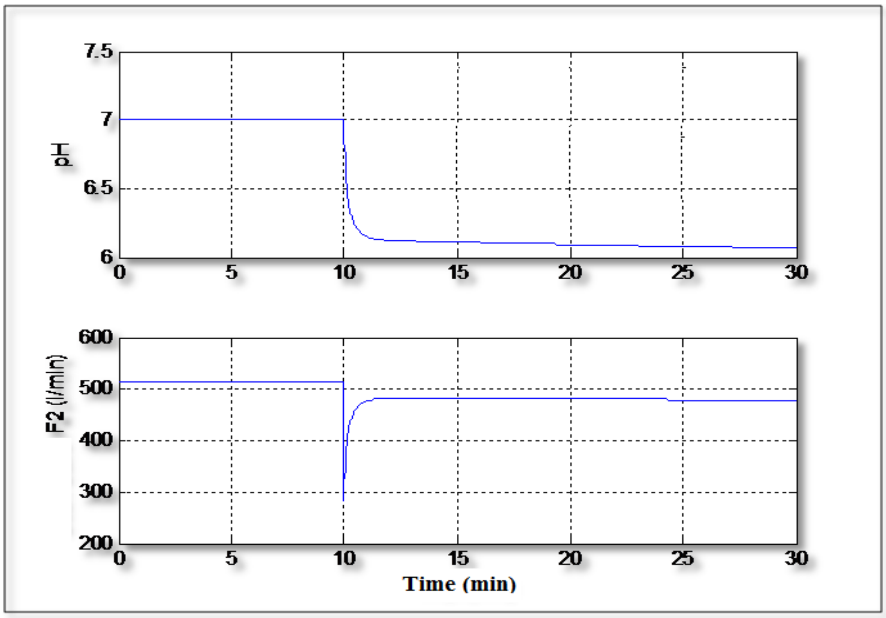

Figure 7. Control of the pH in tracking mode where the value of the setpoint change from 7 to 6 at t = 10 min.

6. Conclusions

This research studied the dynamic and the control of a non-linear pH-CSTR process. The obtained results showed that for the studied process is a first order kind without dead time. Furthermore, the studied process is naturally stable, i.e. it has a certain capacity to regulate itself. The controller can handle the disturbance and it can regulate the pH to its setpoint value and the signal control varies regularly without excessive activity. Furthermore, the controller can handle easily the variation of the setpoint value, in tracking mode, and the signal control varies regularly without excessive variations. This study highlighted the design of a PID controller who was able to regulate the pH despite the occurrence of a high disturbance and the controller was also able to operate in asservissement or tracking mode.

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