Control Techniques Applied to a Nonlinear pH Neutralization Reactor

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Abstract

In this work, the performance of classical PID, IMC and SP controllers are compared with an emerging control technique such as fuzzy logic control. For this purpose, the focus of this work has been on the control strategies of a pH neutralization reactor. The latter is a system that presents high nonlinearities. The results indicated that both classical and fuzzy logic controllers could achieve the objectiveof reaching the desired values, with and without disturbances. However, the difference between the controllers occurs in the settling time, being thus that the fuzzy logic controller presents the fastestand most efficient response. Despite what is indicated by the performance indexes analyzed.

Keywords—pH neutralization reactor, PID control, internal model control, smith predictor control, fuzzy logic control,

DOI Number: 10.14704/nq.2022.20.9.NQ440127 **Neuro Quantology 2022; 20(9):1129-1137**

I. INTRODUCTION

The hydrogen potential (pH) of a solution is defined as the negative decimal algorithm of the hydrogen ion concentration and the control of this variable consists of maintaining it at a certain value [1]; for the case of neutralization processes,the pH control consists of maintaining it at a value equal to 7 mainly to comply with environmental requirements and quality standards [2]. Different chemical, biological, electrochemical, biotechnological, wastewater treatment, pharmaceutical and chemical processing plants need to correctly control this type of pH neutralization processes with an adequate performance [3], however the main problem of this control is that theneutralization processes present time-varying properties, non-linearities and sensitivity to small perturbations when working near the equivalence point, triggering that pH control is considered one of the greatest challenges within the control of chemical processes [4], leading to the generation of a large amount of research on the control of pH neutralization processes in the last 30 years [2].

The strong nonlinearity of the process is due to the natural presence of dead times and time constants within the system [4]. Research available in literature has suggested that to perform the correct pH control, a continuous control based on the principles of feedback should be used, i.e. to minimize the effective dead time in the control loop [4]. It is necessary the correct analysis of the neutralization curve, which relates the flowrate of the neutralizer with the corresponding pH value of the neutralized stream, since in this way it could be characterized the neutralization process with nonlinearities and in steady-state [1].

The most traditional forms of feedback control are the proportional integral control (PI) and the proportional integral derivative control (PID). However, by the high nonlinearity and time variation that the process has, it is not recommended to perform this control algorithm without modifications [5]. Often, this feedback control is combined with a predictive or preventive control, therefore the measured disturbances are compensated before affecting the process [3]. Feedforward control has also been proposed as a solution, however for that purpose it is necessaryto know all the conditions of the input currents, hence it is not a regular feasible control action [1].

In this paper, new controllers are proposed for the correct control of a pH neutralization plant. They are also defined the conditions of the plant, as well as the respective analysis of its nonlinearity and stability of the system. It has been determined the simplified mathematical model of the controlled plant, followed by the application of three classical control techniques to delve into the control challenge of the pH neutralization plant, those techniques were; (i) a PID controller to see the initial response of the system, (ii) an internal model controller and (iii) the Smith Predictor controller. Then, a fuzzy logic control was applied as an emerging optimization technique for the plant control. Finally, this work presents the simulation results, and a comprehensive discussion of the best control strategies.

II. PH NEUTRALIZATION REACTOR

A. *Description of the problem*

The operation of a plant that has a variable volume reactor is analyzed with a variable and dominant time delay. Inside this reactor a fluid neutralization reaction is carried out. The operation of the process is shown in Fig. 1. It is observed that silver has a basic current flow $q_3(t)$, which is manipulated through a valve, this current is mixed with an acid current flow $q_1(t)$, and it is obtained the output flow $q_4(t)$ which has the required pH value. Additionally, the reactor has a buffer stream $q_2(t)$, which has a constant flow that allows maintaining the pH value insensitive to small additions of acids or bases. Inside the plant there is a pH transmitter, installed 674.5 cm away from the reactor, which is calibrated to operate in a pH range of 2.712 to 10.75, which generates a time delay in the final pH value. Consequently, the latter generates a time delay in the measurement.

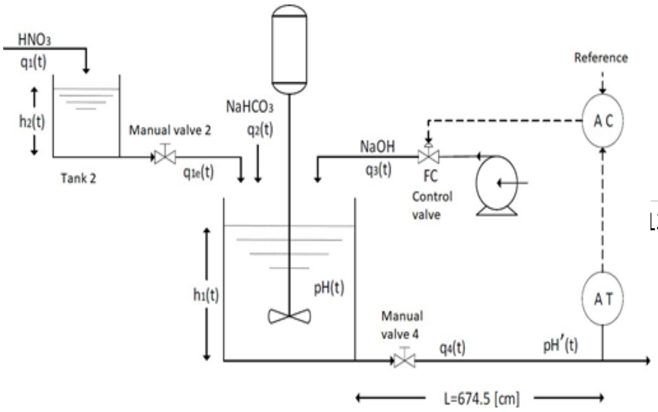

Fig. 1. Diagram of the pH neutralization reactor

The process presents following operational considerations:

- The liquid volume varies without overflowing the reactor.
- The reactor content is well mixed.
- The reactor and piping systems are completely insulated.
- There is assumed complete solubility of the chemical compounds involved.
- The acidic stream $q_1(t)$ presents the major disturbance in the processes.

Equations (1), (2) and (3) show the chemical reactions that are taking place inside the reactor:

$$H_2CO_3 \leftrightarrow HCO_3^- + H^+ \tag{1}$$

$$HCO_3^- \leftrightarrow CO_3^{2-} + H^+ \tag{2}$$

$$H_2O \leftrightarrow OH^- + H^+ \tag{3}$$

Equations (4), (5) and (6) present the relationships between the equilibrium constants.

$$K_{a1} = \frac{[HCO_3^-][H^+]}{H_2CO_3} \tag{4}$$

$$K_{a2} = \frac{[CO_3^{2-}][H^+]}{HCO_3^-} \tag{5}$$

$$K_w = [H^+][OH^-] \tag{6}$$

In order to describe the chemical equilibrium of the process, two invariant reactions named W_a and W_b are introduced for each inflow [5]. W_a is the quantity related to the charge of the ions and W_b is the concentration of the $CO_3{}^{2-}$ ion. *i* ranges from 1 to 4 and it represents all the fluxes. These two reactions are shown in equations (7) and (8).

$$W_{ai} = [H^{+}]_i - [OH^{-}]_i - [HCO_3^{-}]_i - 2[CO_3^{2-}]_i \quad (7)$$

$$W_{bi} = [H_2CO_3]_i - [HCO_3^{-}]_i - [CO_3^{2-}]_i \quad (8)$$

The equations below are describing the dynamic behavior of the process:

$$q_{1e}(t) = C_{V2}\sqrt{h_2(t)} \quad (9)$$

$$q_1(t) = C_{V4}(h_1(t))^n \quad (10)$$

$$q_1(t)\rho - q_{1e}(t)\rho = A_2\rho\frac{dh_2(t)}{dt} \quad (11)$$

$$q_1(t)\rho + q_2(t)\rho + q_3(t)\rho - q_4(t)\rho = A_1\rho\frac{dh_1(t)}{dt} \quad (12)$$

Equations (9) and (10) represent the flow for manual valves 2 and 4, respectively. Equations (11) and (12) correspond to the mass balances of the tank 2 ant the reactor, respectively. ρ is the density, A_i is the cross sectional areas, h_i is the liquid level, C_{Vi} is the flow coefficients and qi(t) is the flow rates of each streams.

B. *System nonlinearities analysis*

The pH neutralization process is highly nonlinear. This is related to the mathematical definition of the hydrogen potential since pH = log [H^+] [6]. Thus, further considerations are:

1) There is an internal state represented by the concentration of hydrogen ions [H^+], which cannot be directly measured [7].
2) It is difficult to record the mass balance in terms of hydrogen and hydroxyl ion concentrations since these variables result from the dissociation and alteration of the electrolyte concentration which is highly variable [8].
3) The logarithmic relationship makes the process very sensitive to small changes in the vicinity of the neutralization point [4].
4) The manipulated variable (i.e., the change of pH as response to the addition of chemical reagents) is highly nonlinear [9].
5) When the system gains are small the closed-loop pH response can be slow, while for high gains the closed-loop pH response can be unstable [7].
6) Variations of inlet flow, reactor volume and mixing rate can lead to variable dead time [9].
7) Under certain conditions, while a decrease in the reagent input flow creates a pH drop, an increment of the flow creates a pH reduction. Thus, in many cases the pH neutralization process shows a nonminimum phase behavior [6].

C. *Stability Analysis*

To perform the system stability analysis, the direct Lyapunov method is used. The solution to the differential equations that describe the process is not required to be explicit. Thus, we proceed with equations (11) and (12), under the following conditions:

$$\begin{gathered} Condition\ 1: \\ q_1 \rightarrow input \\ q_{1e} \rightarrow output \\ \therefore q_1 \geq q_{1e} \end{gathered}$$

$$\begin{gathered} Condition\ 2: \\ q_{1e}, q_2, q_3 \rightarrow input \\ q_4 \rightarrow output \\ \therefore q_{1e} + q_2 + q_3 \geq q_4 \end{gathered}$$

A scalar function is defined in (15), which is based on equations (13) and (14). This function must be positive definite (i.e., greater or equal to zero).

$$\dot{h_1} = \frac{q_1(t)+q_2(t)+q_3(t)-q_4(t)}{A_1}, A_1 > 0 \quad (13)$$

$$\dot{h_2} = \frac{q_1(t)-q_{1e}(t)}{A_2}, A_2 > 0 \quad (14)$$

$$V(h_1, h_2) = \frac{1}{2}h_1^{2-} + \frac{1}{2}h_2^{2-}, h_1, h_2 > 0 \quad (15)$$

The Lyapunov function is derived to satisfy a negative positive condition, such that the stability can be verified. In equation (16), the partial derivative $\dot{V}$ is presented, the latter is less or equal to zero under any condition, validating a negative definite function.

$$\dot{V}(h_1, h_2) = -\frac{1}{h_1^3}\dot{h_1} - \frac{1}{h_2^3}\dot{h_2} \quad (16)$$

$$\dot{V}(h_1, h_2) = -\frac{1}{h_1^3}\left(\frac{q_1(t)+q_2(t)+q_3(t)-q_4(t)}{A_1}\right) - \frac{1}{h_2^3}\left(\frac{q_1(t)-q_{1e}(t)}{A_2}\right) \quad (17)$$

$$\dot{V}(h_1, h_2) = -\frac{q_1(t)+q_2(t)+q_3(t)-q_4(t)}{h_1^3 \cdot A_1} - \frac{q_1(t)-q_{1e}(t)}{h_2^3 \cdot A_2} \quad (18)$$

According to Lyapunov [10], a system is asymptotically stable uniform at equilibrium when: (i) the system is the equilibrium at the origin, (ii) the scalar function V(x) is positive definite, and (iii) the continuous partial derivative $\dot{V}(x)$ is negative definite. The pH neutralization plant, described in this manuscript, complies with conditions 1 and 2. Therefore, it is considered that the physical properties remain global for every scenario. However, when the chemical interaction is analyzed, a buffer effect generated by the dissociation of the electrolyte appears, which produces small amounts of secondary species. These species depend on the electrolyte type and concentrations that are present in the stream. Consequently, the system stability depends on the on the system governing parameters. The latter must be adjusted assuming that the neutralization process is generated at a single point, i.e., when considering the system's chemistry, the stability becomes local [1].

III. CONTROL TECHNIQUES

A. Simplified mathematical model

The simplified mathematical model of the process considers the reaction curve method [11]. This is a technique used to identify dynamic models. Fig. (2) shows the reaction curve obtained under an open-loop operation of the plant, considering a step input, and recording the transmitter output signal. To determine the characteristic parameters (k, τ and t_m) of the First Order Plus Dead Time (FOPDT) system that represents the plant, the Alfaro's two points method was used. Table I shows the values of: p_1 and p_2 which are the percentage values of the change in the system response, and t_1 and t_2 that are the required values of the time.

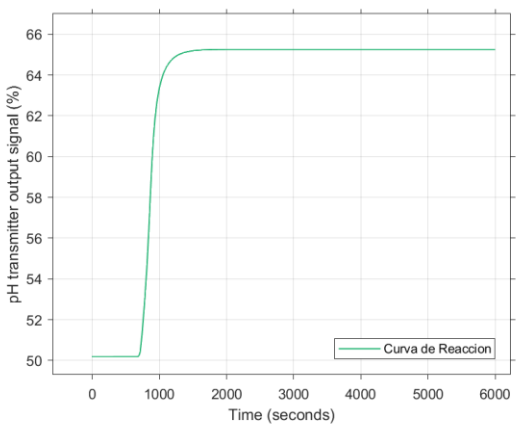

Fig. 2. Process reaction curve

TABLE I
VALUES FOR CHARACTERISTIC PARAMETERS DETERMINATION

$p_1(\%)$	$p_2(\%)$	$t_1(\%)$	$t_2(\%)$
53.94	61.45	405.16	520.15

To obtain the parameters the constants established in Table II are applied with equations (17) and (18). Table III show the characteristics parameters. To obtain the gain, the total change in the output (ΔTO) is divided by the change in the input (ΔCO) as shown in equation (19). The transfer function model of the system using the determined characteristic parameters is presented in equation (20).

TABLE II
CONSTANTS FOR THE IDENTIFICATION OF FIRST-ORDER PLUS DEAD TIME MODELS

a	b	c	d
-0.910	0.910	1.262	-0.262

$$\tau = at_1 + bt_2 \qquad (17)$$
$$t_m = ct_1 + dt_2 \qquad (18)$$

TABLE III
CHARACTERISTIC PARAMETERS OF THE MODEL

τ	t_m
104.6	383.53

$$K = \frac{\Delta TO}{\Delta CO} \qquad (19)$$
$$G_s = \frac{K}{\tau s+1} e^{-t_m s} = \frac{2.9}{104.6s*1} e^{-383.53s} \qquad (20)$$

B. Proportional Integral Derivative Control (PID)

The PID controller is commonly used in industry given its ease of design, simple structure, robust stability and fast response [8]. The control signal used by this controller is presented in (21), and the block diagram is shown in Fig. 3.

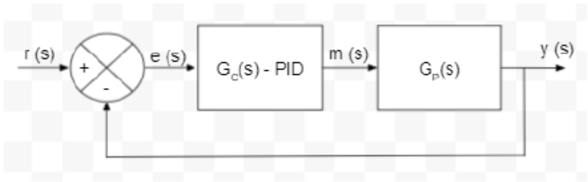

Fig. 3. Block Diagram of PID Controller

In Fig. 3 r(s) is the reference, e(s) is the error, $G_C(s)$ is the transfer function of the PID controller, whose output is m(s) and G_P (s) corresponds to the process whose output is y(s).

$$u(t) = k_P\, e(t)dt + k_I \int e(t)dt + k_D \frac{de(t)}{dt} \qquad (21)$$

In equation (21) e is the error between the desired variable and the calculated variable; and k_P , k_I and k_D are the proportional, integral and derivative gains respectively [12]. The tuning parameters of the PID controller were obtained by Dahlin's method, and the gains are presented in equations (22), (23) and (24):

$$k_P = \frac{1}{2k}\left(\frac{\tau}{t_m}\right) = 0.047 \qquad (22)$$

$$k_I = \frac{k_P}{\tau} = 4.49e^{-4} \qquad (23)$$

$$k_D = k_P \frac{t_m}{2} = 9.013 \qquad (24)$$

C. Internal Model Control (IMC)

For the cases of processes with time delay when working in closed loop, it is necessary to consider more complex controllers than PID that allow intelligent approximations of the time delay term [13]. The internal model control (IMC) is shown in Fig. 4. $G_m(s)$ is the transfer function of the process model and $G_F(s)$ s the transfer function of the controller filter.

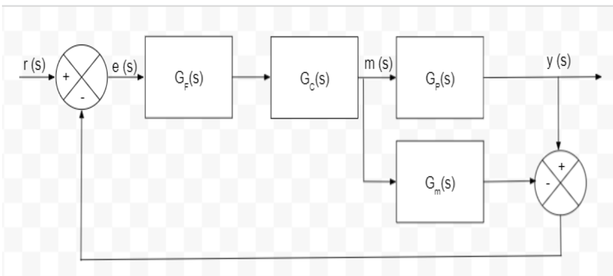

Fig. 4. Block Diagram of Internal Model Control (IMC)

The model that fits the process in some cases may contain terms that are not invertible and therefore would generate unachievable controllers, which is why the model is decomposed into two parts, one invertible, $G_m(s)^-$, and the other noninvertible $G_m(s)^+$, as shown in equations (25), (26), and (27) [14]. This procedure is known as factorization of the model.

$$G_m(s) = G_m(s)^- G_m(s)^+ \qquad (25)$$

where

$$G_m(s)^- = \frac{k}{\tau s+1} = \frac{2.9}{104.6s+1} \qquad (26)$$

$$G_m(s)^+ = e^{-t_m s} = e^{-383.53s} \qquad (27)$$

Following the latter, it is necessary to define the controller $G_C(s)$ exclusively from the invertible part of the model, adding a filter to satisfy the general requirements of increased robustness and noise attenuation specified by the user. In the chemical industry, first order filters are used from the time constant of the open loop system [15]. The transfer function of this controller and the filter are presented in equations (28) and (29) respectively.

$$G_C(s)^- = \frac{\tau s+1}{k} = \frac{104.6s+1}{2.9} \qquad (28)$$

$$G_F(s)^+ = \frac{1}{\tau_f s+1} = \frac{1}{2s+1} \qquad (29)$$

D. Smith Predictor Control (SP)

In industrial process control, most processes are composed of a time constant and a delay, the time delays are usually due to distance rate lags, recycle loops and composition analysis loops [16]. When the delays are small, a PID controller is usually used, but for large delays, the Smith predictor is used [17], which offers a potential improvement in closed-loop performance [18].

The Smith predictor control scheme is shown in Fig. 5 where the process model is divided by separating the delay. This controller normally uses PID type controllers to control the process without dead time. It is called the Predictor because it contains the prediction of X(s) is performed without including the delay time of the process [14]. The parts of the model are presented in (26) and (27), and the PID tuning in (21), (22), (23) and (24).

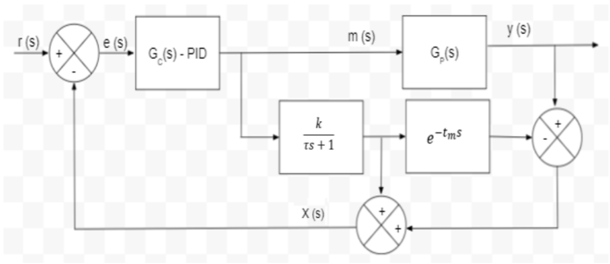

Fig. 5. Block Diagram of Predictor Smith Control (SP)

IV. EMERGING OPTIMIZATION TECHNIQUES – FUZZY CONTROL

Fuzzy logic has two distinct characteristics, the first is to provide a nonlinear relationship induced by membership functions, rules and defuzzification and the second is the human experience which is easily integrated eliminating the need for a mathematical model of the system. It is because of these characteristics that in processes where there is operator experience, this technique can be used over conventional control techniques [1].

A fuzzy logic controller has three main components: the fuzzification of the input signal, a fuzzy engine that handles the inference rules and the defuzzification that generates continuous signals for the actuators. The fuzzification component transforms the input signal into fuzzy linguistic variables. The fuzzy engine performs rule inference based on human experience through linguistic rules. And the defuzzification block converts the inferred control action back into a continuous signal [3].

The development of the fuzzy logic controller can be based on two methodologies: Mamdani and Sugeno, for this work we used Mamdani, which combines practical experience and physical understanding of the process [2]. Most of the fuzzy controllers use as inputs of the controller the control error (e) and the change in the control error i.e. the derivative of the error (Δe), and as output the control signal (u) or its variation (Δu) [3].

The input and output variables, for the control of this process, were considered as triangular membership functions as seen in Fig. 6, with 7 linguistic terms each set in Table IV. Finally, the fuzzy logic control scheme is shown in Fig.6.

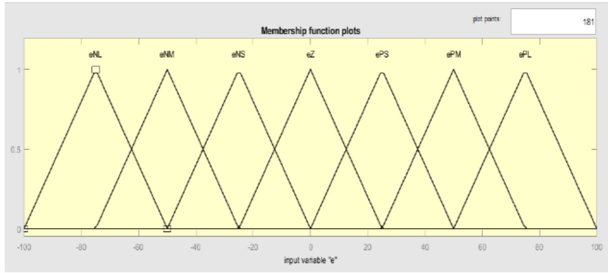

Fig. 6. Example graph of the membership function for the input and output variables of the process

TABLE IV
TERMS OF THE INPUT AND OUTPUT VARIABLES OF THE PROCESS

Term	*Abbreviation*
Negative Large	NL
Negative Medium	NM
Negative SMALL	NS
Positive Large	PL
Positive Medium	PM
Positive SMALL	PS

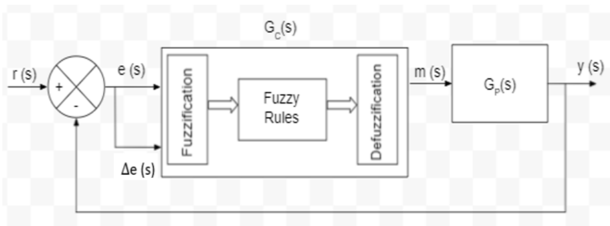

Fig. 7. Block Diagram of Fuzzy Logic Control (FLC)

V. SIMULATION AND RESULTS

A. Response of classical controllers and under the application of an emergent optimization techniquea for the set condition.

The first simulation is presented in Fig. 8 and is performed using a step input, where the output signal of the pH transmitter starts at the reference value of 50.18% and is expected to reach a value of 55%. Three classical control techniques are applied for the pH neutralization reactor: the PID controller, the IMC controller and the Smith Predictor controller, and as an emergent optimization technique, a fuzzy logic controller was applied.

eISSN 1303-5150

In the figure it is observed that the output signal of the PID controller has a settling time of t = 4200s when reaching the desired value, presents a slight over impulse within the allowed values and does not present oscillations in the steady state. The output signal of the IMC controller, on the other hand, has a settling time close to t = 1200s, has a minimum overshoot and a slight oscillation in the transient state. Finally, the signal of the controller with Smith Predictor does not present any overshoot or oscillation in the transient state but has a quite high settling time at t = 5500s. It can be observed that all the applied controllers achieve the desired value. Also, as shown in the figure, the output signal of the fuzzy logic controller does not present over impulses or oscillations in the transient state, and in addition to this has a settling time equal to t = 2000s, i.e. it is a stable and fast controller, unlike the output signals of the classical controllers.

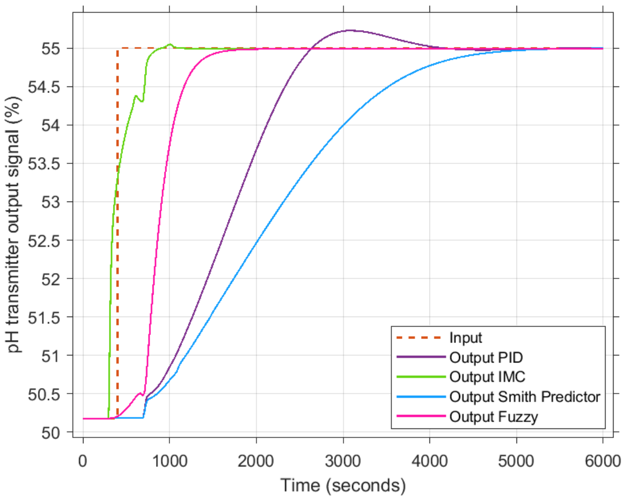

Fig. 8. Transmitter output signal with classical controllers and emerging control techniques

B. Response of controllers with disturbances

The second simulation is presented in Fig. 9 and is performed by keeping the output of the pH transmitter at the reference value of 50.18%. A perturbation was applied to the flow rate of the acid stream $q_1(t)$ at time t = 1000s, this perturbation consisted of changing the flow rate from 16.6 ml/s to 16.8 ml/s. This was followed by another perturbation at t = 5000s, where the flow rate was decreased by 0.1 ml/s, and finally, at t = 10000s, the flow rate was increased again by 0.1 ml/s.

It is observed in Fig. 9 that all controllers allow the system to adjust to the desired pH transmitter reference value (50.18%) after disturbances occur. The output signals of the PID, Smith Predictor and Fuzzy controllers show a decrease in value at t = 2000s before reaching the reference value, however this pH value is within the allowed parameters. After this, at t = 5500s the output signal of these controllers presents a rise peak, caused by the decrease in the flow rate $q_1(t)$. Finally, at t = 11000s, there is a decrease in pH before stabilization, caused by the last perturbation. For the case of the PID controller the settling time of this signal is equal to t = 16000s, for the Smith Predictor controller the settling time is t = 21000s while for the Fuzzy controller the settling signal is lower since the value is t = 12500s. If we observe the output signal of the IMC controller, we can verify that the signal presents an overshoot at t = 1500s approximately, this situation occurs due to the predictive part of the controller, in the same way for the following perturbations an overshoot is presented from t = 5500s to t = 11000s however this impulse is within the allowed values, and in the same way, this signal also reaches stability with a settling time t = 11500s. Therefore, after analyzing the graph, it can be concluded that the fuzzy logic controller has a fast response to disturbances and reaches the desired signal in the shortest settling time.

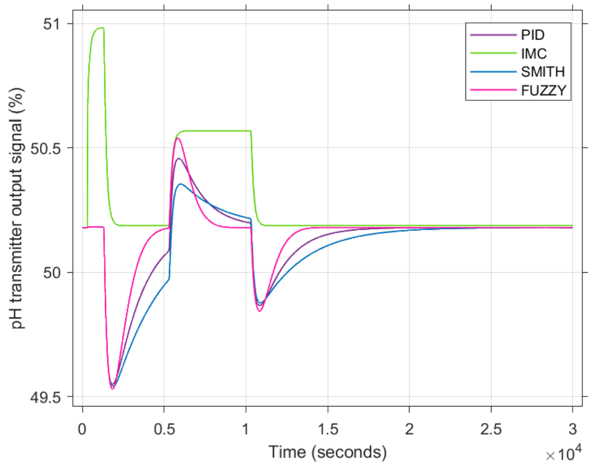

Fig. 9. Transmitter output signal with the different controllers applied

C. Performance analysis between classical controllers and emergent optimization techniques

1) Established condition: To measure the performance of the control techniques presented in this paper, the performance indices ISE and

ISCO were considered, which are indices based on the integral of the square of the error, according to 30. By minimizing these indices, the control error is minimized, improving the performance and thus ensuring a robust optimal control is the result. Table V shows the values corresponding to each index for each controller

$$ISE/ISCO = \int_0^{\infty} e^2(t)dt \qquad (30)$$

TABLE V CONTROLLER PERFORMANCE INDEXES

Controller	ISE	ISCO
PID	2.16e+04	1.27e+05
IMC	1.58e+04	1.12e+05
SP	1.36e+04	1.08e+05
FUZZY	**9.16e+03**	**3.74e+04**

Table VIII shows the values corresponding to each index for each controller, In this case, as shown in the table, the fuzzy logic controller presents the lowest values in both performance indices, so it can be considered that the emergent optimization technique did indeed improve the performance indices, confirming that the fuzzy logic control is an optimal control for the pH neutralization process.

2) Disturbances: The values of the ISE and ISCO performance indices for the controllers when working with the perturbation are presented in Table VI,

The values of the performance indexes ISE and ISCO are presented to compare the classical controllers with the fuzzy logic controller proposed as an emerging control technique, when working with the perturbation. It can be seen, in Table VI that the lowest values of ISE are presented when using the PID controller, however when relating the results of this table with the results of Fig. 9 we can see that this controller has a slow response since its settling time is too high t = 16000s. Likewise, when analyzing Table VI, it is verified that the Fuzzy controller has the lowest ISCO value, a situation that is verified when analyzing Fig. 9, since it is verified that it has a faster response (settling time t = 12500s), so it can be stated that the FUZZY controller can be considered as the most optimal for this plant when it is subjected to disturbances.

TABLE VI
CONTROLLER PERFORMANCE INDEXES

Controller	ISE	ISCO
PID	4.098e+02	9.643e+03
IMC	4.84e+04	5.819e+03
SP	4.571e+02	8.969e+03
FUZZY	6.608e+02	1.023e+03

VI. CONCLUSIONS

The control of the pH neutralization process is one of the most difficult processes to control within the chemical industry, due to the high non-linearity of the system which appears because the pH calculation depends on the concentration of hydrogen ions [H+], which cannot be measured directly. Additionally, as this process has a local chemical stability, i.e. it is subject to the smallest changes within the set parameters, and outside this the system can no longer be controlled because the neutralization reaction does not occur, the control of this process must be carefully tuned.

Due to its functionality and ease of implementation, conventional controllers (PID) have been widely applied to this type of systems, the tuning of the same can be done from the Dahlin equations, after obtaining the simplified model of the plant from the reaction curve; this controller has a slow response to trajectory tracking and the presence of disturbances, however it reaches the desired values. Other classical controllers can also be applied in the control of this process, for example the IMC and the SP; for the tuning of these controllers it is necessary to define again the correct mathematical model of the plant. In the case of the IMC, when disturbances occur, it does not present an adequate response because it presents too abrupt elevations and overshoots in the pH values before reaching the reference, while the SP controller presents a good performance as a controller, which is evidenced in the performance indexes, however, this controller presents a too slow response. Given these drawbacks, an emerging control technique such as the fuzzy logic controller is proposed as an optimization solution, since fuzzy control can be applied to highly nonlinear systems because it is an intelligent control method that mimics human logical thinking and is independent of the exact mathematical model, thus overcoming some of the shortcomings of classical controllers and providing a fast control response.

VII. RECOMMENDATIONS AND FUTURE WORK

For the control of the pH neutralization process it is necessary to work within the established parameters of the chemical reaction, since the chemical stability of the process being local determines that outside these parameters the system cannot be neutralized and therefore its control is non-existent. As future works we propose the use of a controller based on linear algebra (LABC) for the control of this process, since this type of controllers are robust and easy to use when systems have high non-linearities.

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