

Optimal Linear Control Applied to a pH and Volume Control Process: An Economic Feasibility Assessment

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Abstract. This work presents a linear control strategy applied to an agitated tank reactor for pH and volume regulation, based on the linearization of a mathematical model in which both concentration and volume are considered time-varying variables. The linearization is performed around an operating point in order to compute the gains of an LQR controller. Different penalty matrices Q and R are evaluated to obtain different closed-loop plant performances. The pH setpoints were selected according to the Mexican Official Standard NOM-002-SEMARNAT-1996. The simulation results provide evidence of the feasibility of the proposed approach.

Keywords: linear model, state-feedback control, pH control, volume control, LQR, Economic Feasibility

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1 Introduction

In recent years, the scientific community has increasingly focused on the problem of pH control due to its critical role in various industrial processes (Hermansson & Syafie, 2015). This challenge has been approached through multiple control strategies, which can be broadly categorized as nonlinear, linear, and artificial intelligence-based techniques (e.g., fuzzy logic and neural networks).

Among nonlinear control techniques, several studies can be cited. In Ali (2001), an automatically tuned PI algorithm was proposed to stabilize the pH in a neutralization process. The algorithm used a simple process model to predict the closed-loop pH response and its sensitivity to PI settings (note: the volume was not controlled). The simulation results were compared with those obtained from standard PI, gain scheduling (GS), and globally linearizing control (GLC) methods.

Loh et al. (2001) developed a model reference adaptive control scheme was developed to control both pH and liquid level in a continuously stirred tank reactor. The control and parameter estimation laws were derived using a reference model approach suitable for nonlinearly parameterized systems. The proposed controller ensured global stability and zero tracking error for both pH and level variables. Simulation and comparative results were presented, along with experimental results for pH control.

Lee et al. (1999) reported, both numerical and experimental results for the optimal pH control in a batch culture producing curdlan. A fixed operation time of 120 hours was used, and the specific rates of cell growth, substrate consumption, and curdlan production were modeled as functions of pH, sucrose, and ammonium concentrations. These functions were obtained from experiments under constant conditions. The computed optimal pH profile was applied to a batch fermentation process, resulting in a curdlan concentration 78% higher than that achieved under constant pH operation. The optimization was performed using a gradient descent method based on the minimum principle, yielding an open-loop pH profile.

Ashoori et al. (2009) developed a model predictive control (MPC) using a detailed unstructured model for penicillin production in a fed-batch fermenter. The cost function was based on the inverse of penicillin concentration. Simulation results using neuro-fuzzy piecewise linear models were compared with those from an auto-tuned PID controller.

Rakshit and Sahai (1991) enhanced the production of cellulase enzyme using the mutant strain *Trichoderma reesei* E-12, which exhibits partial resistance to catabolite repression. An open-loop optimal pH profile was determined through numerical optimization and semi-empirical modeling. Experimental results showed a 30% increase in enzyme activity and productivity compared to a pH cycling strategy.

Kim et al. (2021) proposed, a two-stage optimal control framework for fed-batch bioreactors. The high-level controller maximized productivity and yield using a nominal model, while the low-level controller addressed real-time disturbances and model-plant mismatches. The framework used Differential Dynamic Programming (DDP) for high-level optimization, and three types of low-level controllers were evaluated: DDP, MPC trajectory tracking, and economic MPC. Simulation results validated the efficiency and necessity of the two-stage approach.

Finally, Wu and Cui (2010) developed a nonlinear model of an overflow neutralization reaction pool. A linearization technique based on the inverse model was applied, and a single closed-loop PI control scheme was implemented using only one actuator. The flow rate of the modulated liquid was used as the main disturbance in the simulation, and the results were presented accordingly.

In this article, linear state-feedback control is used to regulate both the pH and the volume of a tank, starting from given initial pH and volume conditions. A linearized version of the nonlinear plant model is used for controller synthesis; however, the simulation results are obtained using the nonlinear plant model. Unlike other reported results (see Ashoori et al., 2009), the volume in the mathematical model is considered as a variable. Within the framework of classical optimal linear control theory, the synthesis of a linear controller is relatively straightforward. As is well known, standard optimal linear state-feedback control requiring a fixed offset, which may be a disadvantage because it can reduce the robustness of the control scheme. Therefore, an optimal linear control strategy is proposed, avoiding the need to compute such a fixed offset.

Previous studies have addressed pH regulation and, in some cases, the simultaneous control of pH and liquid level in neutralization processes. However, the contribution of the present work does not consist of proposing a new LQR methodology. Instead, this study integrates variable-volume reactor modeling, simultaneous pH and volume regulation, nonlinear closed-loop evaluation, and reagent-consumption analysis within a single framework. Unlike models that assume constant reactor volume, the proposed nonlinear model explicitly considers $V(t)$ as a dynamic state and relates the outlet flow to the liquid volume. Consequently, changes in the inlet flows affect not only the acid–base concentration balance but also the dilution and volume dynamics of the reactor. The LQR controller is synthesized from a local linearization around a specified operating point, whereas its performance is evaluated using the original nonlinear plant model. In addition, different combinations of the weighting matrices Q and R are compared in terms of transient response, acid and base consumption, and associated operating cost. Therefore, the proposed framework allows controller tuning to be examined from both dynamic-performance and resource-utilization perspectives.

To provide a transparent and reproducible assessment of the proposed framework, this study presents the complete derivation of the variable-volume nonlinear CSTR model, the definition of the operating point and deviation variables, the local linearization used for LQR synthesis, and the nonlinear closed-loop simulation procedure. The effects of different weighting matrices are evaluated using both dynamic-performance indicators and reagent-consumption estimates. This integrated analysis is intended to clarify the relationship among mathematical modeling, controller tuning, process performance, and operating cost in pH and volume regulation.

The paper is organized as follows. Section 2 describes the process; Section 3 derives the mathematical model; Section 4 presents the synthesis and simulation of the optimal linear quadratic regulator; Section 5 discusses the economic implications; and the final section provides the conclusions.

2 Description of the Process

The continuous stirred tank reactor (CSTR) is an industrial unit in which chemical reactions take place. In this work, an acid–strong base neutralization reaction is considered. The process involves two inlet flows, $F_1(t)$ and $F_2(t)$, entering the CSTR, and one outlet flow, $F(t)$. Owing to the action of the stirrer, the tank contents are assumed to form a homogeneous mixture, as shown in Figure 1.

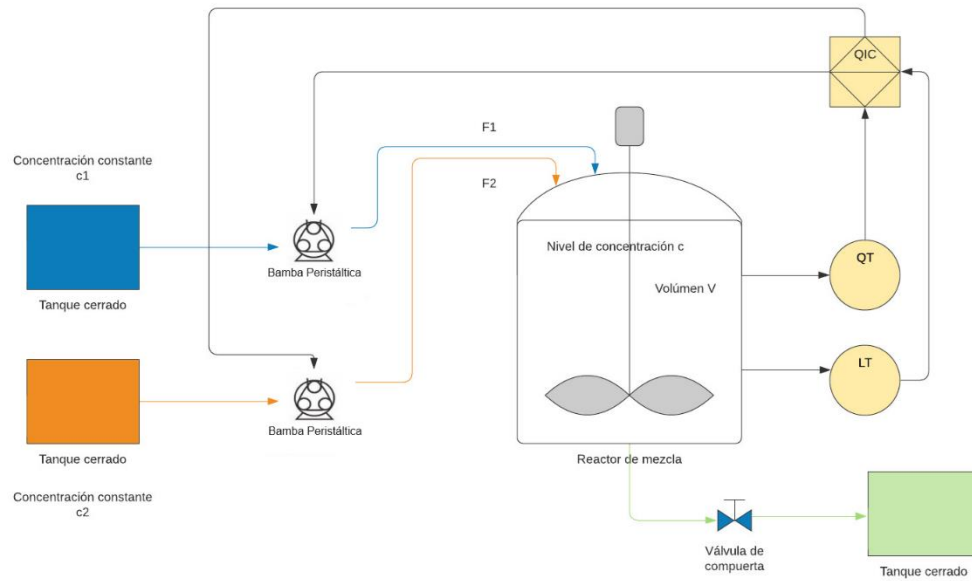


Fig. 1. Process instrumentation diagram

The acidic solution flow $F_1(t)$, consisting of hydrochloric acid (HCl) at a concentration of 0.1 M, enters the tank. The basic solution flow $F_2(t)$, consisting of sodium hydroxide (NaOH) at a concentration of 0.1 M, also enters the tank. The concentration within the CSTR is denoted by β and is assumed to be homogeneous throughout the mixture.

3 Mathematical Model of the Plant

In this section, the nonlinear mathematical model is derived from the process shown in Figure 2, which represents a continuous stirred tank reactor where an acid–base neutralization reaction takes place.

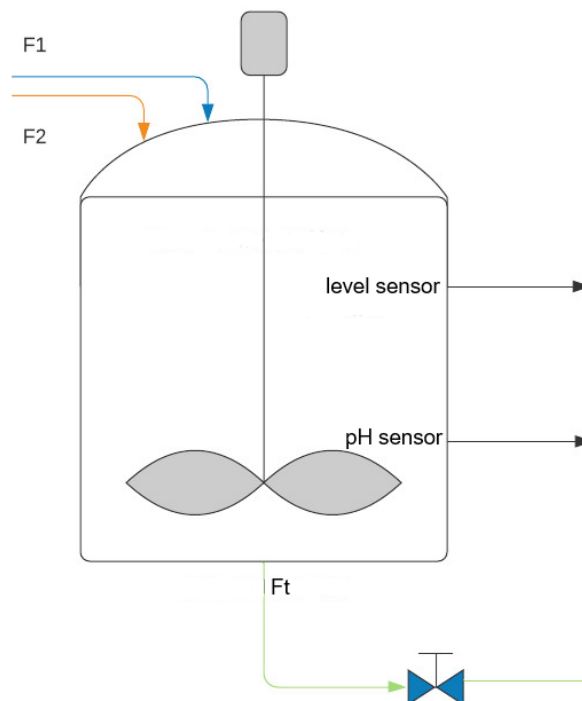


Fig. 2. Continuous stirred tank reactor

The following considerations are taken into account in order to obtain its mathematical model:

- The tank is fed by two time-varying inlet flows, $F_1(t)$ and $F_2(t)$.
- Both feeds dissolve material at fixed concentrations X_{10} and X_{20} .
- The reactor outlet flow is denoted by $F(t)$.
- The tank is assumed to be well stirred; therefore, the concentration of the outlet flow is equal to the concentration $\beta(t)$ of the neutralization product inside the tank.
- All solutions are in an aqueous medium.
- The volume in the tank is defined by $V(t)$.
- The acid and base concentrations within the tank are denoted by X_1 and X_2 , respectively.

The control objective is to regulate volume $V(t)$ and the pH concentration of the liquid inside the tank to predefined setpoints. The measured and regulated variables are volume $V(t)$ and the pH concentration of the liquid in the tank. The manipulated variables are the two time-varying inlet flows, $F_1(t)$ and $F_2(t)$, which can be adjusted by two pumps. Now, consider the mass-continuity equation in the tank (Luyben, 1989):

$$\frac{d(V(t))}{dt} = F_1(t) + F_2(t) - F(t) \quad (1)$$

Here, $V(t)$ is the volume within the tank, $F_1(t)$ and $F_2(t)$ are the input flows and $F(t)$ is the outflow. The equations of component continuity are given as follows (Luyben, 1989):

$$\frac{d(Vx_1)}{dt} = F_1(t)x_{10} - F(t)x_1 \quad (2)$$

$$\frac{d(Vx_2)}{dt} = F_2(t)x_{20} - F(t)x_2 \quad (3)$$

To relate the two variables x_1 and x_2 , $\beta = x_1 - x_2$ is defined; thus, the acid--base neutralization reaction is described by Ali (2001):

$$\frac{d(Vx_1 - Vx_2)}{dt} = F_1(t)x_{10} - F_2(t)x_{20} - F(t)\beta \quad (4)$$

The last equation and equation (1) constitute a well-posed system with two linearly independent state variables. Unlike previous works (see Ali, 2001; Hermansson & Syafie, 2015; Loh et al., 2001), the volume is not assumed to be constant. This assumption allows a more realistic mathematical model to be obtained. In equation (4), if the outlet flow is considered as:

$$F(t) = k_f \sqrt{\frac{V(t)}{S}}$$

follows that the model in state space representation is:

$$\begin{bmatrix} \dot{V}(t) \\ \dot{\beta}(t) \end{bmatrix} = \begin{bmatrix} -\beta(t)k_f \sqrt{\frac{V(t)}{S}} \\ -k_f \sqrt{\frac{V(t)}{S}} \end{bmatrix} + \begin{bmatrix} x_1 & -x_2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} F_1(t) \\ F_2(t) \end{bmatrix} \quad (5)$$

where $V(t)$ is the tank volume, S is the base area of the tank, $F_1(t)$ and $F_2(t)$ are the inlet flows entering the tank, and the constant k_f relates the outlet flow $F(t)$ to the recovery tank.

When a strong acid and a strong base come into contact, a neutralization reaction occurs rapidly. For the CSTR, the mixture is assumed to be homogeneous. If x_1 is considered as $[H^+]$, corresponding to hydronium ions and denoted by CH , and x_2 is considered as $[OH^-]$, corresponding to hydroxyl ions and denoted by COH , the neutralization reaction can be written as:

$$C_H - C_{OH} = x_1 - x_2 \quad (6)$$

From this expression, COH can be obtained and substituted into the equilibrium equation for the ionic product of water, Kw.

$$K_w = [C_H][C_{OH}] \quad (7)$$

This yields the following equation for the concentration of hydronium ions.

$$C_H^2 - (x_1 - x_2)C_H - K_w = 0 \quad (8)$$

Once C_H is obtained, the pH can be calculated using the following expression:

$$pH = -\log_{10}(C_H) \quad (9)$$

In the previous expression, the pH value in the tank is assumed to be known; therefore, CH can be calculated, and the value of x_1 can then be estimated. The value of COH can be obtained from (7), and x_2 can also be estimated. The difficulty of synthesizing nonlinear controllers motivates the evaluation of linear controllers. For this reason, the nonlinear model is linearized in the next section.

3.1 Linearization of the mathematical model

Consider the steady state of the model given by equation (1), where all quantities are constant: F_{10} , F_{20} , and F_0 for the flow rates, V_0 for the volume, and β_0 for the concentration in the tank resulting from the neutralization reaction. Therefore:

$$0 = F_{10} + F_{20} - F_0$$

$$0 = X_{10}F_{10} + X_{20}F_{20} - \beta_0 F_0$$

$$F_0 = k_f \sqrt{\frac{V_0}{S}}$$

The deviation variables are defined as:

$$\mu_1 = F_1(t) - F_{10}$$

$$\mu_2 = F_2(t) - F_{20}$$

$$\delta_1 = V(t) - V_0 \Rightarrow \dot{\delta}_1 = \dot{V}(t)$$

$$\delta_2 = \beta(t) - \beta_0 \Rightarrow \dot{\delta}_2 = \dot{\beta}(t)$$

Using a Taylor series expansion and retaining only the first-order variation, we obtain:

$$\begin{aligned} \dot{\delta}_1 = \dot{V}(t) &\approx F_{10} + F_{20} - k_f \sqrt{\frac{V(t)}{S}} + \frac{\partial}{\partial F_1} \left[F_1 + F_2 - k_f \sqrt{\frac{V(t)}{S}} \right]_{F_1=F_{10}} (F_1 - F_{10}) \\ &+ \frac{\partial}{\partial F_2} \left[F_1 + F_2 - k_f \sqrt{\frac{V(t)}{S}} \right]_{F_2=F_{20}} (F_2 - F_{20}) + \frac{\partial}{\partial V} \left[F_1 + F_2 - k_f \sqrt{\frac{V(t)}{S}} \right]_{V=V_0} (V - V_0) \\ \dot{\delta}_1 = \dot{V}(t) &\approx F_{10} + F_{20} - k_f \sqrt{\frac{V_0}{S}} + \mu_1 + \mu_2 - \frac{k_f}{2V_0} \sqrt{\frac{V_0}{S}} \delta_1 \end{aligned}$$

$$\begin{aligned}
\frac{d(\beta V)}{dt} &\approx \frac{d}{dt} \left[V_0 \beta_0 + \left. \frac{\partial \beta V}{\partial V} \right|_{\substack{\beta=\beta_0 \\ V=V_0}} (V - V_0) + \left. \frac{\partial \beta V}{\partial \beta} \right|_{\substack{\beta=\beta_0 \\ V=V_0}} (\beta - \beta_0) \right] \\
\frac{d(\beta V)}{dt} &\approx \beta_0 \dot{\delta}_1 + V_0 \dot{\delta}_2 \\
\beta_0 \dot{\delta}_1 + V_0 \dot{\delta}_2 &\approx X_{10} \left[F_{10} + \left. \frac{dF_1}{dF_1} \right|_{F_1=F_{10}} (F_1 - F_{10}) \right] - X_{20} \left[F_{20} + \left. \frac{dF_2}{dF_2} \right|_{F_2=F_{20}} (F_2 - F_{20}) \right] \\
&\quad - \frac{k_f}{\sqrt{S}} \left[\beta_0 \sqrt{V_0} + \left. \frac{\partial \beta \sqrt{V}}{\partial \beta} \right|_{\substack{\beta=\beta_0 \\ V=V_0}} (\beta - \beta_0) + \left. \frac{\partial \beta \sqrt{V}}{\partial V} \right|_{\substack{\beta=\beta_0 \\ V=V_0}} (V - V_0) \right] \\
\dot{\delta}_2 = \dot{\beta}(t) &\approx \frac{\mu_1 (X_{10} - \beta_0)}{V_0} - \frac{\mu_2 (X_{20} + \beta_0)}{V_0} - \frac{k(X_{10} - F_0 \delta_1)}{V_0}
\end{aligned}$$

With this linear model, it is possible to obtain an optimal linear controller that regulates the state variables around an operating point.

4 Synthesis of the Optimal Linear Quadratic Regulator

Consider the linear model of the continuous stirred tank reactor.

$$\begin{aligned}
\begin{bmatrix} \dot{\delta}_1 \\ \dot{\delta}_2 \end{bmatrix} &= \begin{bmatrix} -\frac{k_f F_0}{2V_0} & 0 \\ 0 & -\frac{k_f F_0}{2V_0} \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{X_{10} - \beta_0} & \frac{1}{X_{20} + \beta_0} \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \\
y &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}
\end{aligned} \tag{10}$$

The following operating-point parameters are considered:

$$X_{10}=0.1\text{M}; X_{20}=0.1\text{M}; V_0=500 \times 10^{-6} \text{m}^3; \beta_0=2.703 \times 10^{-3} \text{M};$$

$$V_0 = 500 \times 10^{-6} \text{m}^3; F_0 = 3.9894 \times 10^{-6} \text{m}^3/\text{min}; k_f = 175 \times 10^{-5} \text{m}/\text{min}; S = 0.03141$$

$$\begin{aligned}
\begin{bmatrix} \dot{\delta}_1 \\ \dot{\delta}_2 \end{bmatrix} &= \begin{bmatrix} -6.98145 & 0 \\ 0 & -1.3962 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix} + \begin{bmatrix} 1 & 1 \\ 194.594 & -205.406 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \\
y &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}
\end{aligned}$$

The control signal is $u(t) = -Kx(t)$. The optimal feedback gain matrix K is then obtained by minimizing the following quadratic performance index:

$$J = \int_0^\infty \{x^T Q x + u^T R u\} dt$$

As is well known, the first term penalizes state convergence, whereas the second term penalizes the control effort. The matrices satisfy $Q \geq 0$ and $R > 0$. Here, Q and R are selected heuristically as follows:

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; R = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

It is straightforward to verify that the pair (A,B) is controllable. Therefore, the algebraic Riccati equation associated with the linear quadratic regulator problem has a unique solution (Kalman, 1960). Solving the Riccati matrix equation yields the feedback gain matrix K :

$$K = \begin{bmatrix} 0.213 & 0.0914 \\ 0.2071 & -0.9558 \end{bmatrix}$$

The control is:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = - \begin{bmatrix} 0.213 & 0.0914 \\ 0.2071 & -0.9558 \end{bmatrix} \begin{bmatrix} ex_1 \\ ex_2 \end{bmatrix}$$

where

$$ex_1 = V(t) - V_d; \quad ex_2 = \beta(t) - \beta_d$$

Now, these controllers need a fixed offset, this offset was heuristically estimated in both cases (u_1 and u_2). Both offsets guarantee (for this case these offsets represent fixed flows) that the plant remains at the operation point given by the Set Points.

4.1 Simulation of the Optimal Linear Quadratic Regulator

The controller is implemented in the simulated nonlinear model of the agitated tank reactor using MATLAB/Simulink. The results are shown in the sequence of plots.

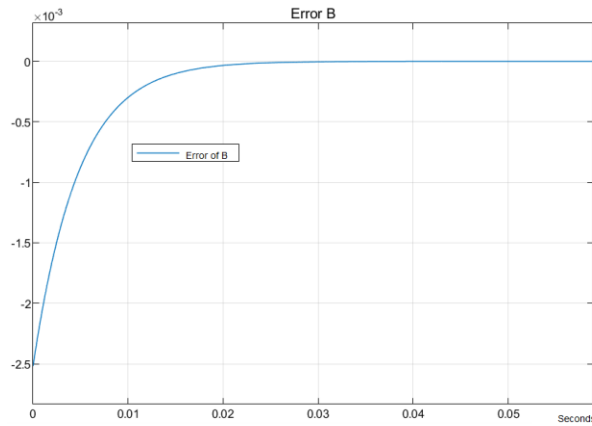


Fig. 3. pH regulation error for a setpoint fixed at 2.9.

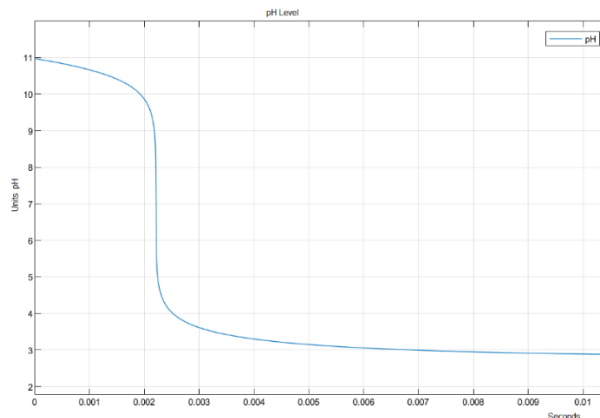


Fig. 4. Dynamic behavior of the pH for a setpoint fixed at 2.9.

As shown in Figures 3 and 4, starting from an initial pH condition of 11 and a setpoint fixed at 2.9, the controller successfully regulates the plant, and the steady-state error converges to zero. The simulation was performed using the nonlinear model controlled by the optimal linear state-feedback law. It should be noted that the initial condition (11 pH units) is not close to the selected setpoint (2.9), which supports the feasibility of the proposed controller. Here the Set Point for the volume was fixed to 600 ml.

5 Economic Implications

Sustainability in the industrial sector is becoming increasingly relevant, as companies must manage their waste responsibly to ensure long-term success and minimize environmental impact. The integration of environmental, social, and governance criteria is essential for sustainable, socially responsible, and environmentally friendly financial performance (Cuellar Hernández et al., 2023).

The determination of pH in industrial wastewater is a critical task for environmental pollution control and management (Secretaría de Medio Ambiente y Recursos Naturales [SEMARNAT], 2022). In Mexico, the determination and control of pH in industrial wastewater are regulated by the Secretaría de Medio Ambiente y Recursos Naturales (SEMARNAT, 2022).

On the other hand, the Mexican Official Standard (Secretaría de Medio Ambiente, Recursos Naturales y Pesca [SEMARNAP], 1998) establishes the maximum permissible limits for contaminants in wastewater discharges to urban or municipal sewerage systems. This standard establishes a permissible pH range of 5.5 to 10 pH units for wastewater discharges, which is essential for sustainable wastewater management in urban areas and for the protection of public health.

The pH values must not fall outside the permissible range in any grab sample; otherwise, the provisions of the General Law on Ecological Balance and Environmental Protection (LGEEPA) apply. According to the Procuraduría Federal de Protección al Ambiente (PROFEPA), economic penalties may be imposed for non-compliance with environmental standards. These penalties may range from the equivalent of 20,000 to 50,000 days of minimum wage in the Federal District at the time the penalty is imposed, corresponding to amounts between MXN 4,148,800.00 and MXN 10,372,000.00 (PROFEPA, s.f.).

The numerical simulation was implemented in MATLAB/Simulink R2020a with the following settings: a stop time of 10 s and a fifth-order Dormand–Prince solver with a fixed step size of 0.00001. The penalty matrices for state convergence (Q) and reagent usage (R) are shown in Table 1. Table 2 presents the operating costs and numerical validation time when the nonlinear mathematical model of the plant is implemented in closed loop with an optimal linear controller. The quadratic performance index uses six different penalty-matrix configurations, Q and R, to reach the volume and pH references in the stirred tank. These references were set to $V_{\text{olde}} = 600$ mL and $\text{pH}_{\text{des}} = 2.9$. The initial conditions of the mathematical plant model were adjusted to realistic values: $V_{\text{olini}} = 500$ mL and $\text{pH}_{\text{ini}} = 8.64$. This initial pH value lies within the allowable range (5.5–10 pH units) for wastewater discharge regulated in Mexico by PROFEPA.

Table 1. Penalty matrices for the quadratic performance index

Penalty matrices Q (convergence)	Penalty matrices R (used reactive quantity)
$Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$R_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$Q_2 = \begin{bmatrix} 50 & 0 \\ 0 & 50 \end{bmatrix}$	$R_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$Q_3 = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}$	$R_3 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$Q_4 = \begin{bmatrix} 0.3 & 0 \\ 0 & 0.3 \end{bmatrix}$	$R_4 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$Q_5 = \begin{bmatrix} 0.008 & 0 \\ 0 & 0.008 \end{bmatrix}$	$R_5 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
$Q_6 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$R_6 = \begin{bmatrix} 500 & 0 \\ 0 & 500 \end{bmatrix}$

Table 2. Total costs (in Mexican pesos) obtained with different penalty matrices ($V_{\text{olde}} = 600$ mL and $\text{pH}_{\text{des}} = 2.9$), considering the unit cost of the reagents.

Q, R	Settling time (s)	Acid volume F1 (L)	Acid cost	Base volume F2 (L)	Base cost	Total cost
Q_1, R_1	1.166	0.2279	\$157.93	1.4254	\$752.61	\$910.55
Q_2, R_2	0.151	0.0296	\$20.51	0.1855	\$97.94	\$118.46
Q_3, R_3	1.745	0.3403	\$235.83	2.1288	\$1,124.01	\$1,359.83
Q_4, R_4	2.324	0.4523	\$313.44	2.8294	\$1,493.92	\$1,807.37
Q_5, R_5	Doesn't reach the reference (587 mL) 26.43	20.1340	\$13,952.86	122.0917	\$64,464.42	\$78,417.28
Q_6, R_6	Doesn't reach the reference (586 mL) 29.042	22.0866	\$15,306.01	133.887	\$70,692.34	\$85,998.35

As is well known in optimal control theory, penalty matrices characterize different controllers, which may exhibit distinct behaviors in the plant response. However, Table 2 reports on the different costs obtained from the six penalty configurations considered in the performance index. These results provide evidence that different penalties lead not only to distinct closed-loop temporal responses of the plant, but also to a significant economic and ecological impact. Indeed, penalty configurations 5 and 6 show not only a waste of reagents without achieving the desired regulatory pH levels, but also a considerable use of economic resources. This demonstrates how modern control theory can influence the optimization not only of traditional control parameters, such as settling time, overshoot, and peak time, but also of the resources employed.

6 Conclusions

In the present article, unlike previous results, the mathematical model has been modified to account for variable volume, and a linear optimal control strategy was considered to close the loop with the nonlinear reactor model within a specified operating region. For the synthesis of the optimal linear quadratic regulator, different penalty matrices associated with state convergence and control effort were considered in the quadratic performance index. The economic impact of using the six different penalty configurations was assessed by calculating the volumes, in liters, of the acid and base reagents considered in the numerical simulation. The evidence obtained highlights the importance of proper tuning in optimal control, while also showing that numerical simulation can help identify significant economic savings prior to practical implementation.

The contribution of this study is not the development of a new LQR algorithm, but the integration of a variable-volume nonlinear CSTR model, simultaneous pH and volume regulation, nonlinear closed-loop simulation, and reagent-consumption assessment. The results indicate that the selection of the weighting matrices Q and R affects not only the transient response of the controlled process but also the quantities of acid and base required to reach the desired operating conditions. Thus, LQR tuning should be evaluated by considering both conventional control-performance criteria and resource-utilization implications.

The results presented in this study should be interpreted as a simulation-based evaluation of the proposed modeling and control framework. Although the nonlinear simulations provide evidence of the effectiveness of the controller within the analyzed operating conditions, further work should include experimental validation, actuator constraints, sensor dynamics, process disturbances, and parameter uncertainty. These extensions are necessary to assess the practical implementation and robustness of the proposed approach in an actual wastewater-treatment process.

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