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Research Article

Partial Control of a Continuous Bioreactor: Application to an Anaerobic System for Heavy Metal Removal

M. I. Neria-González,[1] P. A. López-Pérez,[2] and R. Aguilar-López[3]

[1] *Chemical & Biochemical Engineering Division, Tecnológico de Estudios Superiores de Ecatepec, Avenida Tecnologico S/N, Valle de Anahuac, 55210 Ecatepec de Morelos, MEX, Mexico*
[2] *Escuela Superior de Apan, Universidad Autónoma del Estado de Hidalgo, Carretera Apan-Calpulalpan, Km 8, Chimalpa Tlalayote S/N, Colonia Chamilpa, 43900 Apan, HGO, Mexico*
[3] *Biotechnology and Bioengineering Department, CINVESTAV-IPN, Avenida Instituto Politécnico Nacional 2508, San Pedro Zacatenco, 07360 Mexico City, MEX, Mexico*

Correspondence should be addressed to R. Aguilar-López; raguilar@cinvestav.mx

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This work presents a control strategy for a continuous bioreactor for heavy metal removal. For this aim, regulation of the sulfate concentration, which is considered the measured and controlled state variable, allowed diminishing the cadmium concentration in the bioreactor, where the corresponding controller was designed via nonlinear bounded function. Furthermore, a nonlinear controllability analysis was done, which proved the closed-loop instability of the inner or uncontrolled dynamics of the bioreactor. A mathematical model, experimentally corroborated for cadmium removal, was employed as a benchmark for the proposed controller. Numerical experiments clearly illustrated the successful implementation of this methodology; therefore, cadmium removal amounted to more than 99%, when the initial cadmium concentration was up to 170 mg/L in continuous operating mode.

1. Introduction

Attention to bioremediation processes has greatly increased during the last decade. Anaerobic reduction has been used as a means for treating a variety of sulfate-containing industrial water generated from various industrial activities, such as food processing, pulp and paper industries, mining and mineral processing, scrubbing of flue gases, and petrochemical industries [1]. Moreover, the existing sulfate can be reduced to hydrogen sulfide resulting in unfavorable ecological effects. Therefore, the use of biological sulfate reduction (BSR) is an attractive alternative or supplement for the simultaneous removal of heavy metals and sulfate from wastewaters. In BSR, the produced sulfide forms insoluble precipitates with the metal ions; the extremely low solubility of the formed sulfide metal (bioprecipitation) allows for the removal of heavy metals from the wastewater [2, 3].

To achieve the full biological potential of cells, optimal environmental conditions for cell growth and product formation must be maintained in the bioreactor, at least, regarding the most important key parameters. The wide use of anaerobic sulfate-reducing bioreactors has been addressing the necessity of robust, flexible, and efficient operation modes, where the corresponding control strategies play key roles. The anaerobic sulfate-reducing systems are affected by many factors, including temperature, retention time, pH, and chemical composition of the wastewater [4, 5]. Much emphasis has been placed on the control of continuous and fed-batch bioreactors because of their traditional prevalence in industry; however, if production of cell mass or product is to be optimized, then continuous operation is desirable for the development of bioprocess engineering. Unforeseen disturbances in a continuous bioreactor may result in a failure in the reactor's operation, which requires a new start-up procedure.

The key objective of a continuous bioreactor control system is usually washout; this can be avoided by closing one feedback loop and controlling cell mass or substrate concentrations. Besides, to optimize the reaction and maintain

the quality of the product, it could be essential to keep biomass, substrate, and some products at desired values [6, 7]. To this date, PID-type controllers are the most applied in the process industries. However, because of (i) rapid development in biotechnology, (ii) the computational capabilities of controllers, (iii) the industrial demands, (iv) process optimization in upscaling, and (v) complexity of biosystems, control actions have had to be increased, so the challenge is to implement advanced control algorithms [8, 9].

A number of papers, dealing with the new controller design under the framework of gain scheduling, have been published in the open literature dealing with predictive, optimal, and nonlinear control theories [10, 11]. Unfortunately, because of their mathematical complexity, most of them cannot be applied to industrial plants. In order to solve this problem, control engineers have had to design *ad hoc* control schemes to be able to deal with demanding operating conditions. For example, Aguilar et al. [12] have proposed novel approaches to design nonlinear PI- and PID-type controllers using more sophisticated techniques that allow developing new friendly tuning rules for the controller's gains and assuring semiglobal robust performance. Another successful control approach is related to sliding mode, which shows some robust properties against model uncertainties and external disturbances when the system reaches the named sliding surface; however, the chattering problem can induce, in the worst case, system's instabilities. A way to avoid the above chattering is the use of high order sliding-mode controllers, which have been proposed to provide smoothness performance to the corresponding output injection and improve the closed-loop system behavior; however, the theoretical frame to prove closed-loop convergence is complex [13]. Under this frame, a class of sigmoid functions has been proposed to substitute the discontinuous terms of the sliding-mode controllers [14]. In order to solve the problems described, in this paper, a class of nonlinear controller with bounded output feedback is proposed to provide stabilization for a class of continuous sulfate-reducing bioreactor. This model was employed as a benchmark system to implement a nonlinear controller, where the corresponding feedback is related to bound sigmoid functions. Furthermore, a nonlinear controllability analysis was done. Bioreactor regulation was achieved via sulfate concentration, which is considered as the measured and controlled state variable; this allowed diminishing the cadmium concentration in the bioreactor. Besides, a theoretical frame of the closed-loop stability was provided, which ensured loop stability.

2. Materials and Methods

The presented model was based on a previous work of López-Pérez et al. [15]. The strain *Desulfovibrio alaskensis* 6SR was used [16]. Inoculation and analysis procedures and media used have been described elsewhere [17–19]. The proposed model considers the inhibitory effect of cadmium and H_2S on microbial growth. Furthermore, the model includes four processes: (1) carbon source consumption, (2) microbial sulfate reduction, (3) biofilm formation, and (4) cadmium removal. The mathematical model describes the kinetics of cadmium removal in batch systems. A straightforward estimate of acetate production with lactate consumption was obtained by the combination of the Moser-Boulton models and biomass concentration, according to (1) and (2). The Levenspiel inhibition model was modified to describe the reduction of sulfate; the classical growth with the reduction of sulfate to H_2S is described by (3)–(5). The mass balance, describing the biofilm formation, is given by (6). The mass balance describing the removal of cadmium is specified by a modified Levenspiel-Haldane model [20] (see (7)). Therefore, the mathematical model of the bioreactor can be expressed by

lactate mass balance (γ_L) as follows:

$$\frac{d\gamma_L}{dt} = D\left(\gamma_{L_{\text{in}}} - \gamma_L\right) - K_{LA}Y_{L/X}\left[\frac{K_{\text{ace}}}{\gamma_A + K_{\text{ace}}}\right]\left[\frac{\gamma_L^{\delta}}{K_{\text{lac}} + \gamma_L^{\delta}}\right]\gamma_X, \tag{1}$$

acetate mass balance (γ_A) as follows:

$$\frac{d\gamma_A}{dt} = -D\gamma_A + K_{LA}Y_{A/X}\left[\frac{K_{\text{ace}}}{\gamma_A + K_{\text{ace}}}\right]\left[\frac{\gamma_L^{\delta}}{K_{\text{lac}} + \gamma_L^{\delta}}\right]\gamma_X, \tag{2}$$

sulfate mass balance ($\gamma_{SO_4^{-2}}$) as follows:

$$\frac{d\gamma_{SO_4^{-2}}}{dt} = D\left(\gamma_{SO_{4\text{in}}^{-2}} - \gamma_{SO_4^{-2}}\right) - \frac{K_{\text{spx}}}{Y}\left[1 - \frac{\gamma_{H_2S}}{K_P}\right]^{\alpha}\left[\frac{\delta_{SO_4^{-2}}}{K_S + \gamma_{SO_4^{-2}}}\right]\gamma_X\gamma_L^{\varepsilon}, \tag{3}$$

biomass balance (γ_X) as follows:

$$\frac{d\gamma_X}{dt} = -D\gamma_X + K_{\text{spx}}\left[1 - \frac{\gamma_{H_2S}}{K_P}\right]^{\alpha}\left[\frac{\delta_{SO_4^{-2}}}{K_S + \gamma_{SO_4^{-2}}}\right] \cdot \left[1 - \frac{\gamma_{\text{Cdl}}}{K_{\text{Cdl}}}\right]^{\beta}\gamma_X\gamma_L^{\rho} - K_d\gamma_X\gamma_L^{\rho}, \tag{4}$$

sulfide mass balance (γ_{H_2S}) as follows:

$$\frac{d\gamma_{H_2S}}{dt} = -D\gamma_{H_2S} + \frac{K_{\text{spx}}}{Y_P}\left[1 - \frac{\gamma_{H_2S}}{K_P}\right]^{\alpha}\left[\frac{\gamma_{SO_4^{-2}}}{K_S + \gamma_{SO_4^{-2}}}\right]\gamma_X\gamma_L^{\varepsilon}, \tag{5}$$

biofilm mass balance (γ_B) as follows:

$$\frac{d\gamma_B}{dt} = -D\gamma_B + K_{\text{bio}}\left[1 - \frac{\gamma_B}{K_B}\right]^{\beta}\gamma_X\gamma_L, \tag{6}$$

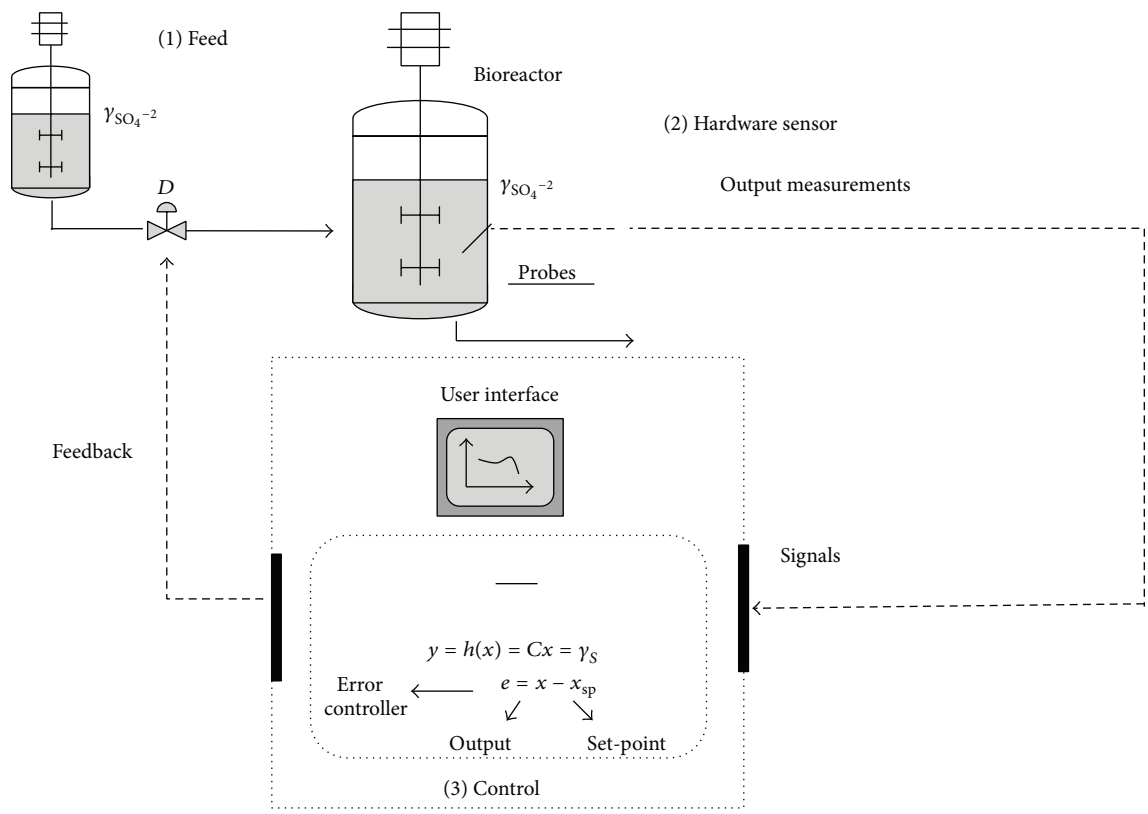

Figure 1: Proposed controller architecture.

cadmium in liquid form mass balance (γ_{Cdl}) as follows:

$$\frac{d\gamma_{\text{Cdl}}}{dt} = D\left(\gamma_{\text{Cdl}_{\text{in}}} - \gamma_{\text{Cdl}}\right) - K_{\text{Cdl}}\left[1 - \frac{\gamma_{\text{H}_2\text{S}}}{K_{\text{spx}}}\right]^{\theta}\left[\frac{\gamma_{\text{Cdl}}}{K_1 + \gamma_{\text{Cdl}} + \gamma_{\text{Cdl}}^2/K_2}\right]\gamma_X\gamma_B. \quad (7)$$

Here, γ, α, and β are the exponential terms of the Luong model; ε is the exponential term for lactate concentration; θ and δ are the exponential terms of the Moser model; D is the dilution rate; K_d is the mortality constant; Cdl_{in} is the initial cadmium concentration; K_1 is the saturation coefficient; and K_2 is the inhibition constant for Haldane; Y is the yield constant; K_S is the Monod saturation constant for sulfate (SO_4^{-2}); K_P is the inhibition constant for nondissipated hydrogen sulfide (H_2S); K_{lac} is the inhibition parameter of lactate; K_{ace} is the inhibition parameter of acetate; K_{Cdl} is the inhibition constant for cadmium; $Y_{L/X}$ is the lactate/biomass yield coefficient; $Y_{A/X}$ is the acetate/biomass yield coefficient.

3. Controller Design

This methodology allows regulating γ_S to a desired set point; therefore, regulation is achieved via sulfate concentration, which is considered the measured and controlled state variable; this allows diminishing the cadmium concentration in the bioreactor, where the corresponding feedback is related to the given dilution rate (input flow) (see Figure 1).

Let us consider a generalized space state representation of systems (1)–(7):

$$\dot{X} = f(x) + g(x)u, \quad (8)$$

$$y = h(X) = CX, \quad (9)$$

where $X = [\gamma_L, \gamma_A, \gamma_S, \gamma_X, \gamma_{\text{H}_2\text{S}}, \gamma_B, \gamma_{\text{Cdl}}]$ is the corresponding state vector, y is the output, u is the vector control input, $f(x)$ is a nonlinear, continuously differentiable vector field, and $g(x)$ is an invertible matrix.

Now, consider the set $\Omega \subset \mathscr{R}^7$; therefore,

$$\begin{aligned}
\Omega = \Big\{&\left(\gamma_L, \gamma_A, \gamma_S, \gamma_X, \gamma_{\text{H}_2\text{S}}, \gamma_B, \gamma_{\text{Cdl}}\right) \in \mathscr{R}_+^7 \mid 0 \le \gamma_L \\
&\le \gamma_{\text{in}};\ 0 \le \gamma_A \le \gamma_{A_{\max}};\ 0 \le \gamma_S \le \gamma_{S_{\text{in}}};\ 0 \le \gamma_X \\
&\le \gamma_{X_{\max}};\ 0 \le \gamma_P \le \gamma_{P_{\max}};\ 0 \le \gamma_B \le \gamma_{B_{\max}};\ 0 \le \gamma_{\text{Cdl}} \\
&\le \gamma_{\text{Cdl}_{\text{in}}}\Big\}, \qquad (10)\\
f(x) &\in C^{\infty};\\
f(0) &= 0;\\
\|g(x)\| &\le G \quad \forall x \in \mathscr{R}_+^7, \text{ where } G < \infty.
\end{aligned}$$

Let us assume x_{sp} as the desired trajectory, sp means set point, and $y = \gamma_S$.

Defining the vector error as $e(t) = x - x_{sp}$ and $e(t) = x - x_{sp}$, therefore $\dot{e} = \dot{x} - \dot{x}_{sp}$; here, it is considered that $\dot{x}_{sp} = f(x_{sp})$; this means that the proposed trajectory obeys the mass conservation principle under the action of the considered control law. From the above, the corresponding equation for the control error dynamics is as follows:

$$\dot{e} = f(x) - f\left(x_{sp}\right) + g(x)u. \tag{11}$$

Because the system is physically bounded (there are no infinite concentrations), the following assumption is considered:

(A1) $\|f(x) - f(x_{sp})\| \leq \ell\|x - x_{sp}\|$; that is, the system is Lipschitz bounded.

Condition (A1) can be fully satisfied if the following supremum is finite:

$$\ell \coloneqq \sup_{x\in\Omega} \left\| f'(x) \right\|, \tag{12}$$

where $f'(x)$ is the Jacobian matrix of the vector field $f(x)$ and $\|\cdot\|$ is the Euclidian norm.

Proposition 1. *Suppose that $x(t)$ is defined for all $t \geq 0$, and (A1) is satisfied. The control input is proposed as follows:*

$$u = k_0\left(\frac{e}{1+e}\right) * \operatorname{sign}(e) + k_1 e, \tag{13}$$

where

$$\operatorname{sign} = \begin{cases} 1 & \text{if } e > 0 \\ \text{undefined} & \text{if } e = 0 \\ -1 & \text{if } e < 0, \end{cases} \tag{14}$$

where k_0 and k_1 are the corresponding controller's gains.

Then, the estimation error is bounded by $\|e(t)\| \leq k_0 G/\ell$.

Sketch of Proof. To prove the closed loop of the proposed controller, let us consider the dynamic equation of the control error ($e = x - x_{sp}$), as follows:

$$\begin{aligned} \dot{e} = f(x) - \Bigg(& f\left(x_{sp}\right) \\ & - g(x)\left(k_0\left(\frac{e}{1+e}\right) * \operatorname{sign}(e) + k_1 e\right)\Bigg). \end{aligned} \tag{15}$$

Considering the Cauchy-Schwarz inequality to (15) by applying (A1), the quota for the error was obtained as follows:

$$\|\dot{e}\| \leq (\ell - Gk_1)\|e\| + Gk_0\left\|\left(\frac{e}{1+e}\right) * \operatorname{sign}(e)\right\|. \tag{16}$$

Therefore, (16) can be rewritten as follows:

$$\|\dot{e}\| \leq (\ell - Gk_1)\|e\| + Gk_0. \tag{17}$$

Consider that the term $\|\circ\| \leq 1$ because its argument belongs to a class of sigmoid function.

By solving (17) and considering $(\ell - Gk_1) < 0$ for $t \to \infty$, by a proper selection of the control's gain k_1, it can be concluded that the control error belongs to a closed ball $\|e(t)\| \leq Gk_0/\ell$; that is, there exists a closed set $B_R(0)$ with radius $R \leq Gk_0/\ell$, where all trajectories of $e(t)$ remain inside.

4. Internal Dynamics for Nonlinear System

Now, to analyze the inner dynamics of a system, it is necessary to find the dynamics of its inverse [21]. For nonlinear systems, fulfillment of this inverse process is often impossible. However, for control affine systems that are partially controlled, it is possible to assess stability features of the zero dynamics when the system is regulated by the control of a subset of q states x_{co}, following the dynamics of the (n-q) uncontrolled states x_{un} (18):

$$\begin{gathered} \dot{x} = f(x) + g(x)u \longrightarrow \\ \begin{cases} \dot{x}_{co} = f_{co}(x) + g_{co}(x)U \\ \dot{x}_{un} = f_{un}(x) + g_{un}(x)U. \end{cases} \end{gathered} \tag{18}$$

Here, $x_{co} \in \mathfrak{R}^q$, $f_{co}(x) \equiv \{f_{co} : \mathfrak{R}^n \to \mathfrak{R}^q\}$, $g_{co}(x) \equiv \{g_{co} : \mathfrak{R}^n \to \mathfrak{R}^q\}$, $x_{un} \in \mathfrak{R}^{n\text{-}q}$, $f_{un}(x) \equiv \{f_{un} : \mathfrak{R}^n \to \mathfrak{R}^{z\text{-}q}\}$, and $g_{un}(x) \equiv \{g_{un} : \mathfrak{R}^n \to \mathfrak{R}^{n\text{-}q}\}$.

Now, it is necessary to find theoretical values of manipulated input, U, assuming that the regulated variables will remain steady at the desired set point as a consequence of the control action (9). If the evolution of the dynamic behavior of the uncontrolled variables x_{un} (20) is not stable, it is possible to conclude that the zero dynamic is neither stable [21]; hence, the control will exhibit poor performance during closed-loop operation:

$$\begin{aligned} \dot{x}_{co}^{sp}(t) = 0 \Longleftrightarrow u^{sp} = & -\left[g_{co}^T(x(t))\, g_{co}(x(t))\right]^{-1} \\ & \cdot g_{co}^T(x(t))\, f_{co}(x(t)) \end{aligned} \tag{19}$$

$$\begin{aligned} \Longrightarrow \dot{x}_{un}(t) = & f_{un}(x(t)) - g_{un}(x(t)) \\ & \cdot \left[g_{co}^T(x(t))\, g_{co}(x(t))\right]^{-1} g_{co}^T(x(t))\, f_{co}(x(t)). \end{aligned} \tag{20}$$

Therefore, all the balance for the uncontrolled variables should tend to an attractor in order to ensure complete stability of the zero dynamics and, of course, the control at the desired set point. The policy proposed is to ask for all the balance $\dot{x}_{un}(t)$ to exhibit a negative sign (decreasing trend) when operating at the set point.

Defining $x_{un} = \left[x_{un1}\ x_{un2}\ \cdots\ x_{un,n\text{-}q}\right]^T$, $x_{un}^{sp} = \left[x_{un1}^{sp}\ x_{un2}^{sp}\ \cdots\ x_{un,n\text{-}q}^{sp}\right]^T$ with $x_{un,i} \geq x_{un,i}^{sp}$. The controller of the system $\dot{x}$ will be stable $\forall t > 0$, if and only if $\dot{x}_{un} \leq 0$, $\forall x_{un} \in \mathfrak{R}^{n\text{-}q}$ (see [22]).

5. Results and Discussion

Numerical simulations were done employing the 23s Matlab™ R2009 library to solve ordinary differential equations. The

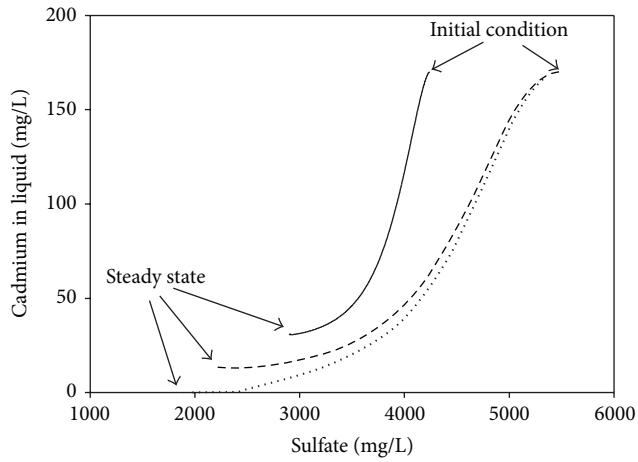

Figure 2: Phase diagram of the cadmium in liquid-sulfate transition.

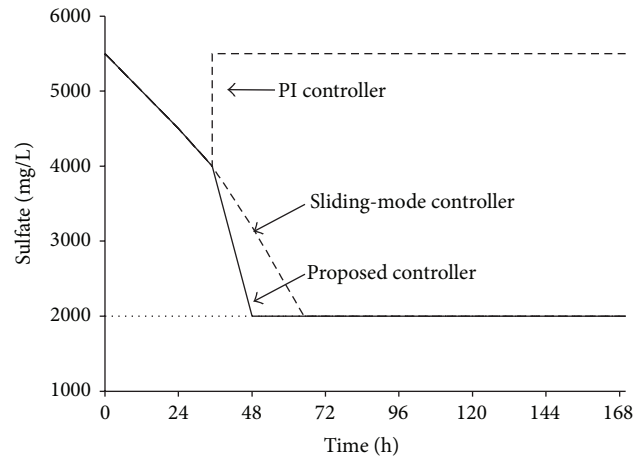

Figure 3: Closed-loop performance of the sulfate concentration.

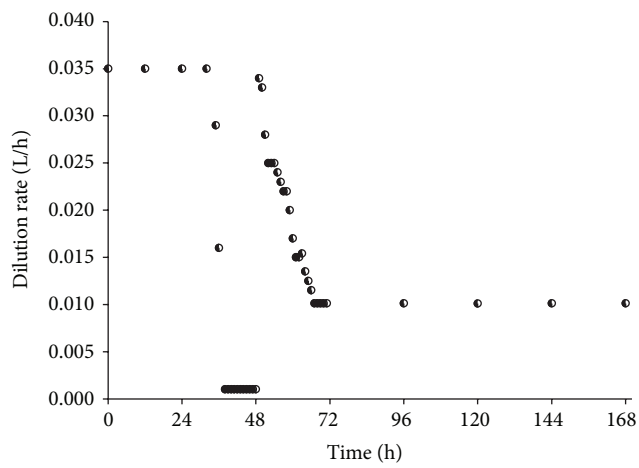

Figure 4: Control effort.

initial conditions for the corresponding concentrations were considered as $\gamma_{SO_4^{-2}0} = 5000$ mg/L, $\gamma_{H_2S0} = 15$ mg/L, $\gamma_{X0} = 150$ mg/L, $\gamma_{L0} = 4250$ mg/L, $\gamma_{A0} = 5$ mg/L, $\gamma_{B0} = 0.5$ mg/L, and $\gamma_{Cdl0} = 170$ mg/L. The anaerobic bioreactor model is simulated to evaluate the benefits of the proposed control law through comparison between open-loop and closed-loop performances. The local stability analysis of the bioreactor was determined for a dilution rate $D = 0.035$ L/h, for which the corresponding eigenvalues were $\lambda_S = -0.02$, $\lambda_P = -0.24$, $\lambda_X = -0.19$, $\lambda_L = -0.02$, $\lambda_A = -0.02$, $\lambda_B = -0.04$, and $\lambda_{Cdl} = -0.033$; from the above, it can be concluded that the corresponding steady state is locally stable according to Lyapunov criteria [23].

Considering that sulfate concentration can be measured easily via spectrometric devices, it is considered as the corresponding measured system output and the controlled variable [24]. Dynamic interactions among variables play important roles in control action; hence, multiple stationary states will be detected in the system. Figure 2 shows the effect of the initial sulfate concentration on the removal of cadmium.

Therefore, the aim of the simulation was to select the concentration of sulfate to reach a cadmium concentration below 0.05 mg/L; hence, the desired concentration was 1400 mg/L of residual sulfate. This analysis led to indirect removal of cadmium in liquid form via bioprecipitation, taking as reference the following reaction mechanism:

$$SO_4^{-2} + 8e^- + 4H_2O \longrightarrow S^{-2} + 8OH^- \tag{21}$$

$$\underset{\text{sulfide}}{S^{-2}} + \underset{\text{heavy metal |soluble|}}{M^{+2}} \longrightarrow \underset{\text{heavy metal |insoluble|}}{MS\downarrow} \tag{22}$$

At the beginning of the simulation, the bioreactor was conducted in an open-loop operation and then the controller was on. For comparison purposes, a well-tuned linear PI and sliding-mode controller were implemented too. For the linear PI controller, the corresponding gains were $K_P = 1.9$ and $K_P/\tau_I = 0.9$, whereas the controller's gain for the sliding mode was $K_{\text{sliding}} = 1.9$.

Figure 3 shows the close-loop performance of the controlled variable (sulfate) for the regulation case. A fast response of the system can be seen when the controller acted and forced the trajectory to the desired set point; on the contrary, the performances of the sliding-mode and PI controllers were not satisfactory because the set point was not reached; this situation is clearly reflected by the behavior of the control effort shown in Figure 4.

Note that the sulfate concentration set point leads the cadmium concentration to the desirable levels given by the environmental regulations (lower than 0.05 mg/L), which is the main task of this process; therefore, cadmium removal amounted to more than 99%, when its initial concentration was 170 mg/L, in continuous operating mode (Figure 5).

Finally, Figure 6 shows the result of zero dynamics; these dynamics of nonlinear systems indicate the stability properties of the closed system when the output is forced to be zero [22]. Thus, it is essential to assure that uncontrolled states reach a stable or unstable behavior. Figure 6(a) shows a negative behavior of uncontrolled variables that tend to stabilize (sulfide, biomass, and biofilm). It should be noted that the time-derivatives converge to zero for cadmium,

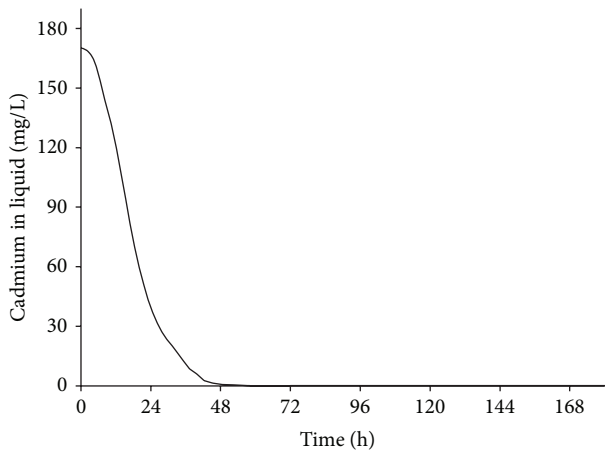

Figure 5: Performance of the uncontrolled cadmium concentration.

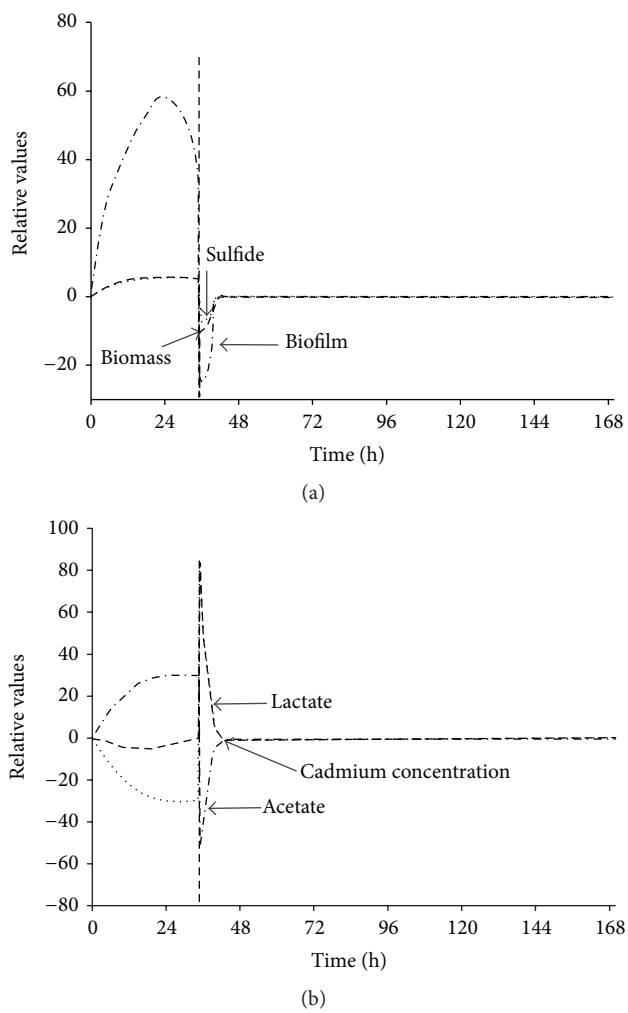

Figure 6: The zero dynamics performance of the uncontrolled states.

lactate, and acetate concentrations, therefore stabilizing the concentration of cadmium (Figure 6(b)).

6. Concluding Remarks

In this paper, we propose a new approach to control sulfate concentration in an anaerobic bioreactor. The selected sulfate concentration set point led indirectly to a diminution of cadmium concentration low enough to agree with environmental regulations. The control strategy is based on the feedback sigmoid functions. The presented controller was tested by computer simulations on a nonlinear model of a continuous anaerobic bioreactor for cadmium removal purposes. Simulation results demonstrated the applicability of the presented control strategy and its usefulness, especially for performance comparison with proportional integral (PI) and sliding-mode controllers.

Competing Interests

The authors declare that they have no competing interests.

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