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Research Article

Chaos Suppression via Euler-Lagrange Control Design for a Class of Chemical Reacting System

Ricardo Aguilar-López

Department of Biotechnology and Bioengineering, Centro de Investigación y de Estudios Avanzados del I.P.N. (CINVESTAV), Av. Instituto Politécnico Nacional, No. 2508, Colonia San Pedro Zacatenco, C.P. 07360, Ciudad de México, Mexico

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

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In this work the problem of chaos suppression for a class of continuous chemical reactor with chaotic dynamics is tackled via a nonlinear control strategy. The proposed controller is developed under the framework of optimal control theory, where a functional is proposed to maximize the chemical reaction rate via a proposed Lagrangian-type which contains directly the state equation of the reacting system, avoiding the problems of Lagrange, the Hamiltonian formulation, and consequently the explicit constraints to the system. This allows solving in an easier form the optimization problem in comparison with the standard methods. This procedure allows suppressing the chaotic behavior of the reacting system by stabilizing the reaction rate term by leading it to an extreme value. Numerical experiments are done in order to show the satisfactory performance of the proposed methodology.

1. Introduction

The stabilization of nonlinear systems with complex or chaotic behavior has been analyzed from several years ago. In particular, the stabilization via nonlinear controllers with regulation purposes in chemical reactors is also a classical task for processes engineers; the control of chemical reactors has been done via linear PID, adaptive, predictive, I/O linearizing, fuzzy, neural, and optimal controllers with success [1–6]. A widely employed control strategy is related to the optimal control theory, considering external or without constraints. For improved reactor operation, the need to implement optimal operational trajectories, which include maximum productivity and optimal cost, for example, leaded to the tracking trajectory control problem, where the optimal control designs have been successful [7–10]. In optimal control approach, the Hamiltonian techniques have been applied to nonlinear processes, where the corresponding Hamiltonian equations must be developed to include nonlinear constraints and construct an adequate functional which is named objective function; in order to obtain a controller for the required task, as common in optimal control theory, here the Pontryagin's maximum (or minimum) principle is used to find the best possible control for taking a dynamical system from one state to another, especially in the presence of constraints for the state variables and input controls [10]. Also, in optimal control theory the corresponding functional (objective function) to be maximizing or minimized only contains in its structure nonlinear terms of the state variables and the control input in order to generate a control law design for a specific purpose. In this work a Lagrangian based directly on the state equation of the chemical reactor with chaotic behavior is proposed, in order to develop a functional to stabilize the reactor's operation in a critical point the reaction rate, suppressing the complex oscillations in the process.

2. Control Design

The fundamental framework of the optimal control theory lies on the calculus of variations, which is related to the basic trajectory optimization problem, where a functional $\mathcal{F}(\mathcal{L}(\bullet)) \coloneqq \mathbb{R}^q \longrightarrow \mathbb{R}$ is a scalar cost function or cost index or performance index, which needs to be maximizing or minimizing; this objective is reached by solving the corresponding Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial x_1} - \frac{d}{dx_2}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}_1}\right) = 0 \tag{1}$$

The term $\mathscr{L}$ is known as the Lagrangian of the system under study.

In general the cost functional $\mathscr{F}$ can be represented as

$$\mathscr{F} = \psi\left(x_f, t_f\right) + \int_{t_0}^{t_f} \mathscr{L}\left(t, x, u\right) dt \tag{2}$$

where $\psi(x_f, t_f)$ is an algebraic term to be minimized (or maximized) at final conditions, subject to the following constraints:

(i)

$$\dot{x} \coloneqq \frac{dx}{dt} = f\left(x\right) + g\left(x\right) u \tag{3}$$

The above equation is the state equation.

Here, $x \in \mathbb{R}^n$ is the state variable vector, $f(x) : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a nonlinear vector field, where $f(x) \subset \Sigma \in C^{\infty}$ and Σ is a compact set, $g(x)$ is a smooth and invertible bounded function, and $u \in \mathbb{R}^m$, with $m \leq n$ is the control input.

(ii)

$$\omega\left(x_f, t_f\right) = 0 \tag{4}$$

The vector ω represents the terminal constraints.

(iii)

$$x\left(t_0\right) = x_0 \tag{5}$$

which represent the initial conditions.

The case related to the solving of (2) subject to constraints (2)–(5) is known as the Problem of Bolza [11, 12]. Particular cases, where the functional is defined as $\mathscr{F} = \psi(x_f, t_f)$ or $\mathscr{F} = \int_{t_0}^{t_f} \mathscr{L}(t, x, u)dt$ subject to the same constraints (2)-(5), are classified as the Problem of Mayer or the Problem of Lagrange, respectively [13, 14].

Note that the solutions of the above-mentioned problems can be complex given the nonlinear nature of the cost functional and the corresponding constraints; an alternative methodology consists of avoiding the nonlinear constraints by incorporating them to the cost functional via the Hamiltonian formulation [8], which is an augmented cost functional with the following structure:

$$\begin{aligned}\mathscr{F} = {} & \psi\left(x_f, t_f\right) \\ & + \int_{t_0}^{t_f} \left(\mathscr{L}\left(t, x, u\right) + \lambda^T \left[f\left(x\right), u - \dot{x}\right]\right) dt\end{aligned} \tag{6}$$

As mentioned above, the solution of (6) also can be complex by the highly nonlinearities of the augmented functional.

Now, let us consider the following functional form:

$$\mathscr{F}\left(\mathscr{L}\right) = \int_0^T \mathscr{L}\left(x, \dot{x}, u\right) dt \tag{7}$$

Now, it is needed to determine the extreme value of functional (7); therefore,

$$\delta\mathscr{F}\left(\mathscr{L}\right) = \int_0^T \delta\mathscr{L}\left(x, \dot{x}, u\right) dt \tag{8}$$

The differential form of the corresponding Lagrangian $\mathscr{L}$ is giving by

$$\delta\mathscr{L}\left(x, \dot{x}, u\right) = \frac{\partial\mathscr{L}}{\partial x}\delta x + \frac{\partial\mathscr{L}}{\partial\dot{x}}\delta\dot{x} + \frac{\partial\mathscr{L}}{\partial u}\delta u \tag{9}$$

Substituting (9) into (8),

$$\delta\mathscr{F}\left(\mathscr{L}\right) = \int_0^T \left(\frac{\partial\mathscr{L}}{\partial x}\delta x + \frac{\partial\mathscr{L}}{\partial\dot{x}}\delta\dot{x} + \frac{\partial\mathscr{L}}{\partial u}\delta u\right) dt \tag{10}$$

The following terms of the differential form of the Lagrangian are now represented as

$$\frac{\partial\mathscr{L}}{\partial x}\delta x = \frac{\partial\mathscr{L}}{\partial x}\delta x\frac{\delta u}{\delta u} = \frac{\partial\mathscr{L}}{\partial x}\frac{\delta u}{u'} \tag{11}$$

where

$$\frac{\delta u}{\delta x} \coloneqq u' \tag{12}$$

and integrating by parts

$$\int_0^T \frac{\partial\mathscr{L}}{\partial\dot{x}}\delta\dot{x}\, dt = \frac{\partial\mathscr{L}}{\partial\dot{x}}\,\delta x\Big|_0^T - \int_0^T \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{x}}\right)\delta x\, dt \tag{13}$$

Now, from (3) the following is considered:

$$f\left(x\right) = \dot{x} - g\left(x\right) u \tag{14}$$

The particular Lagrangian for (7) is proposed as

$$\mathscr{L}\left(x, \dot{x}, u\right) \equiv \dot{x} - g\left(x\right) u \tag{15}$$

Note that the proposed Lagrangian only contains information of the corresponding state equation of the system under study.

Therefore, from (15) and (10)

$$\begin{aligned}\frac{\partial\mathscr{L}}{\partial x} &= -g'\left(x\right) u; \\ \frac{\partial\mathscr{L}}{\partial\dot{x}} &= 1; \\ \frac{\partial\mathscr{L}}{\partial u} &= -g\left(x\right)\end{aligned} \tag{16}$$

Then

$$\int_0^T \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{x}}\right)\delta\dot{x}\, dt = 0 \tag{17}$$

$$\frac{\partial\mathscr{L}}{\partial\dot{x}}\,\delta x\Big|_0^T = 0 \tag{18}$$

because $\delta x|_0 = 0$ and $\delta x|_T = 0$.

Finally, from (9), (10), and (16)-(18)

$$\frac{\delta\mathscr{F}\left(\mathscr{L}\right)}{\delta u} = \int_0^T \left(\frac{u}{u'}g'\left(x\right) + g\left(x\right)\right) dt \tag{19}$$

The extreme value of functional (19) is then determined by the following restriction:

$$\frac{\delta\mathscr{F}\left(\mathscr{L}\right)}{\delta u} = 0 \tag{20}$$

Equivalently,

$$\delta\mathscr{L}\left(x, \dot{x}, u\right) = \frac{u}{u'}g'\left(x\right) + g\left(x\right) = 0 \tag{21}$$

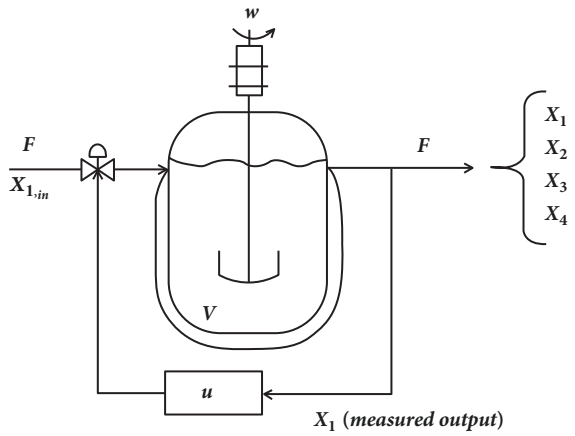

Figure 1: Scheme of the operation of the continuous chemical reactor.

From (21), the differential equation to describe the corresponding control law u to stabilize the system (3) in an extreme point can be obtained, without considering any explicit constraints, as follows:

$$u' = -\frac{g'(x)}{g(x)}u \tag{22}$$

Solving (22),

$$u(x) = u_0 \exp\left(\int_0^T -\frac{g'(x(t))}{g(x(t))}dt\right) \tag{23}$$

where u_0 is the initial condition of (22).

3. Application Example

From several years ago experimental evidence of chaotic behavior in chemical reacting systems exists, since the corresponding chemical species act as reactive, intermediates, and products, where reversible and autocatalytic chemical paths are generally present and hyperchaotic dynamics can undoubtedly be found [15, 16]. In particular, the chemical reactors are process equipment designed to produce high value compounds or products from the corresponding reactions via a chemical transformation, to reach this important objective, process analysis must be performed in order to determinate steady-states multiplicity, open-loop instabilities between others, to select under thermodynamic and kinetic restrictions, the optimal operating regions which maximize the reactor's productivity, process security, and operation cost, where the closed-loop operation is frequently needed to keep the reactor's variables in the selected set points. The continuous reactor operation consists of a multicomponent inlet flow F, which feeds the chemical reactions to the process equipment; the corresponding chemical reactions are carried out inside the reactor with a multicomponent output flow, where a specific set of state variables (x_1 in this case) can be measured to give feedback to the control algorithm and generate the control actions by the corresponding actuator, in this case the control valve, as can be observed in Figure 1.

If the control input u is assumed constant with a nominal value, the corresponding operation is in open-loop regimen. The main task of the control input is to compensate via the input flow manipulation, the residence time in the chemical reactor under the proposed control law (see (23)) to reach an extremum seeking of the corresponding reaction rate.

In particular, the mathematical model presented by [17] is considered, where, via mass conservation principle, a four-state dynamics system is proposed. For the kinetic model developing, several assumptions are considered; the chemical reactions are carried out in perfect homogeneous conditions in a well stirred tank reactor under isothermal operation, first-order kinetic is considered for the reactions from X_4 to X_1 and X_2 and X_1 to X_2, the reactive X_1 catalyzes the production of the compound X_3, the two reactions from X_1 are catalyzed by X_2 and X_3, the reaction from X_4 is also catalyzed by X_3, and all the chemical species are involved in autocatalytic reactions and they are mathematically modeled by Michaelis-Menten structures [17].

The following general chemical kinetic pathway is proposed:

$$\begin{aligned} X_1 &\longrightarrow X_1^* \longrightarrow X_2 + X_3 \\ X_1 &\longleftrightarrow X_4 \longrightarrow X_2 \\ X_2 &\longrightarrow 2X_2^* \longrightarrow Product \\ X_3 &\longrightarrow 2X_3^* \longrightarrow Product \\ X_4 &\longrightarrow 2X_4^* \longrightarrow X_3 + Product \end{aligned} \tag{24}$$

where X_i^* for i= 1, 2, 3, 4 are the corresponding activate chemical complexes, which are assumed in pseudo steady state, as usual.

This kinetic model is extended to continuous reactor's operation, showing complex (chaotic) oscillations. The mathematical model is represented by the following set of nonlinear ordinary differential equations and represents the mass balances for each one of the chemical compounds in terms of the corresponding mass concentrations.

Mass Balances

$$\begin{aligned} \dot{x}_1 = {} & d_0 + k_8 x_4 - k_1 \frac{x_1 x_2}{x_1 + K} - k_2 \frac{x_1 x_3}{x_1 + K} \\ & + (x_{1,in} - x_1) u \end{aligned} \tag{25}$$

$$\dot{x}_2 = k_3 x_1 + k_4 x_2 + k_9 x_4 - k_5 \frac{x_2}{x_2 + K} + (x_{2,in} - x_2) u \tag{26}$$

$$\dot{x}_3 = d_1 + k_6 x_1 x_3 - k_7 x_3 + (x_{3,in} - x_3) u \tag{27}$$

$$\dot{x}_4 = (k_{10} - k_8 - k_9) x_4 - k_{11} \frac{x_3 x_4}{x_4 + K} + (x_{4,in} - x_4) u \tag{28}$$

Here, $x = [x_1 \ x_2 \ x_3 \ x_4]$ is the vector of mass concentrations. The set of kinetic parameters is given as follows: k_1 = 1.0; k_2 = 1.0; k_3 = 1.0; k_4 = 0.25; k_5 = 152.5; k_6 = 1.0; k_7 = 130; k_8 = 0.001; k_9 = 1.0; k_{10} = 1.051; k_{11} = 0.5; K = 0.001. The inlet concentrations to the reactor are as follows: $x_{1,in}$ = 150;

$x_{2,in} = x_{3,in} = x_{4,in} = 0$, and the nominal value of the control input is considered as $u = 0.015$. The corresponding initial conditions are x_{10} =129.1; x_{20} = 76.06; x_{30} = 0.5895; and x_{40} = 21.38, d_0 =90; d_1 = 2.2 are constant disturbances which are included to simulate realistic process operation. As usual for this processes, let us consider that the control input is defined as $u = F/V$, where F is the volumetric inlet flow and V is the volume of the reactor, which is assumed as constant as usual for this systems.

Now, for this application case, let us consider the state equation (21) to construct the corresponding Lagrangian:

$$\mathcal{F}(\mathcal{L}) = \int_0^T \left(\dot{x}_1 - \left(x_{1,in} - x_1\right) u\right) dt \tag{29}$$

Taking into account (14), note that

$$f(x) = d_0 + k_8 x_4 - k_1 \frac{x_1 x_2}{x_1 + K} - k_2 \frac{x_1 x_3}{x_1 + K} \tag{30}$$

Here:

$$g(x) = \left(x_{1,in} - x_1\right) \tag{31}$$

As observed, (31) represents the input and output mass flows, where

$$g'(x) = -1 \tag{32}$$

Applying (31)-(32) to (23), the corresponding control law is giving by

$$u(x) = \left(x_{1,in} - x_1\right)^{-u_0} \tag{33}$$

Noting the simple structure of the resulting controller, the controller's structure is properly model free and only needs online measurements of the state variable x_1 and some parameters as the inlet concentration $x_{1,in}$ and the initial condition of the control input u_0; these parameters are easily available for the standard operation of this kind of process; these characteristics would allow its real time implementation.

4. Results and Discussion

Numerical experiments were done in order to show the performance of the proposed control strategy. The numerical simulations were carried out employing ODE 23s Matlab library to solve the dynamic model of the chemical reactor, under the parametric and initial conditions described above. In this analysis a Single-Input Single Output (SISO) closed-loop operation is considered, where the state equation to be controlled corresponds to the state variable x_1. Firstly, the open-loop behavior of the bioreactor shown in Figures 2–5 observed the complex (chaotic) oscillations in the corresponding time series and the phase portraits; as previously reported in [17], the system keep positive Lyapunov indexes confirming the complexity of the oscillations. In order to show the performance of the proposed methodology, the proposed controller is activated at $t = 100$; here the effect of

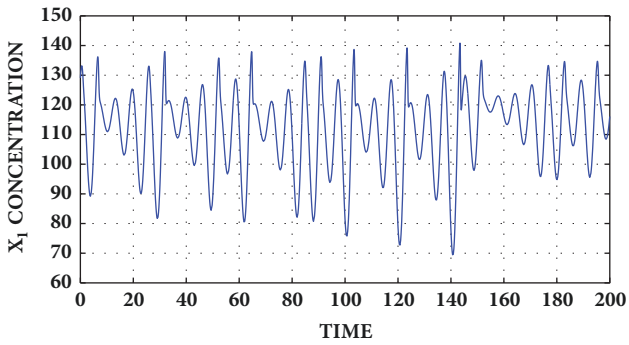

Figure 2: Open-loop dynamic behavior of the mass concentration of x_1.

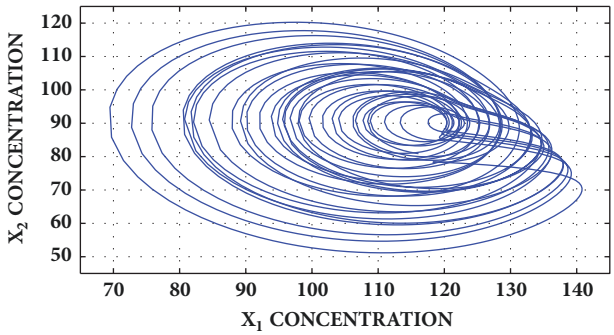

Figure 3: Open-loop 2D phase portrait.

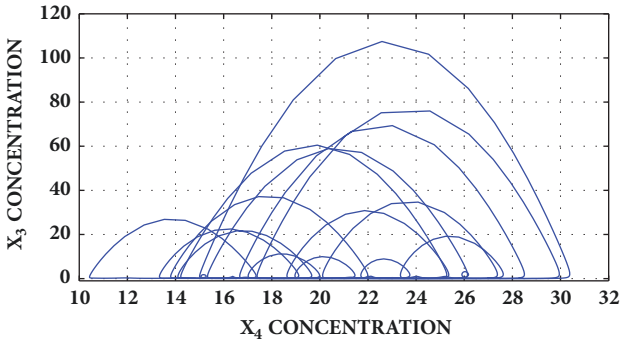

Figure 4: Open-loop 2D phase portrait.

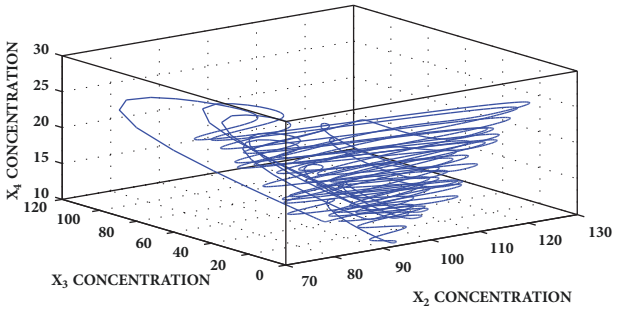

Figure 5: Open-loop 3D phase portrait.

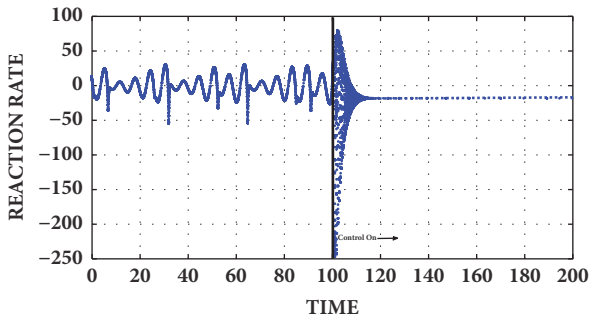

Figure 6: Open-loop and closed-loop dynamic behavior of the reaction rate.

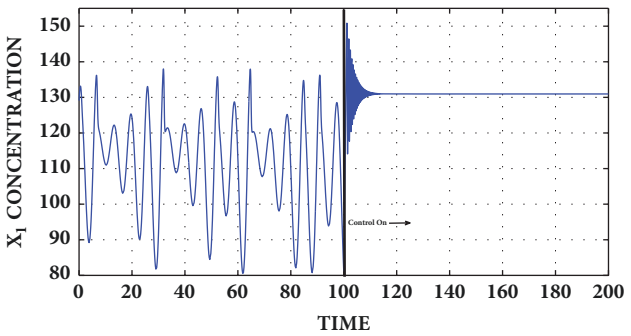

Figure 7: Open-loop and closed-loop dynamic behavior of the mass concentration of x_1.

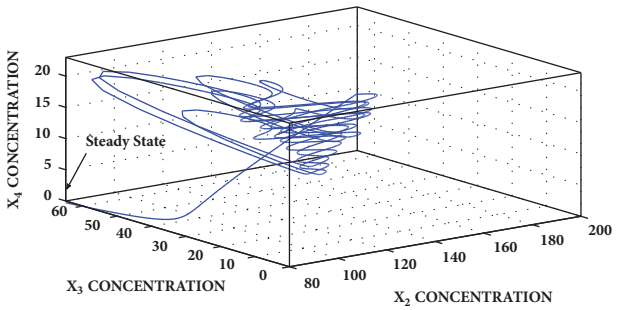

Figure 8: Closed-loop 3D phase portrait.

the control action in the corresponding reaction rate term is observed; Figure 6 shows that the oscillating behavior is suppressed after an overshot and a settling time of 15 time units, reaching to a stable and constant value of -20 units in the reaction rate; therefore, Figure 7 shows the corresponding effect in the mass concentration of the chemical specie x_1 which increase to a fixed value to 131.7 units; this is an important issue such that this means that the corresponding reaction rate term is maximized by the proposed controller as expected and in accordance with the corresponding design. Figure 8 is related to the closed-loop behavior of the trajectories in a 3D phase portrait, where the change in the trajectory is observed in comparison with the open-loop behavior; furthermore, in Figure 9 the control effort under the proposed controller is observed; notice that the control action acts almost immediately, with a small overshoot,

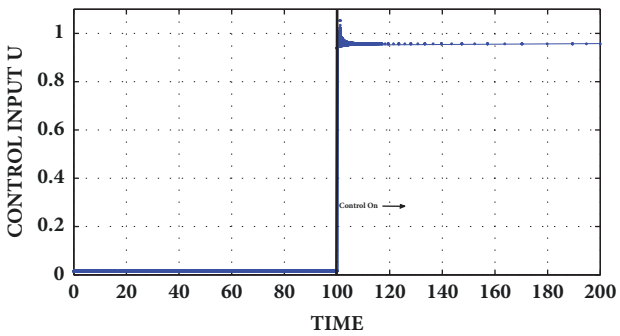

Figure 9: Control Input effort.

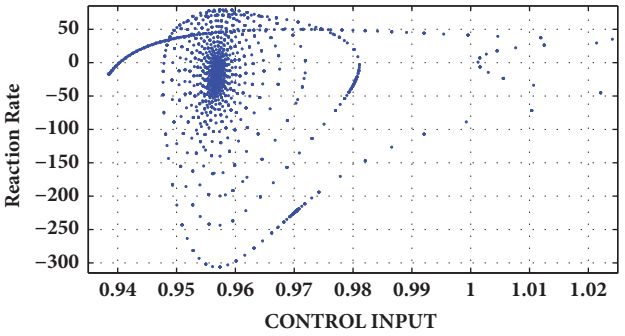

Figure 10: Reaction rate behavior versus control input action.

increasing its value and reaching the corresponding steady state with realizable values. On the other hand, Figure 10 is related to the evolution of the reaction rate term as a function of the control input, as presented in the functional structure of (23) and (33), and it can be seen that the reaction rate reaches a stable equilibrium point $f(x_{eq})$ = -20, at u = 0.957, in accordance with the previous figures.

5. Concluding Remarks

In this work an optimal control strategy to suppress the chaotic behavior of a class of continuous chemical reactor is presented. The proposed methodology is based on a Lagrangian structure which includes directly the corresponding state equations of the system under analysis, avoiding the inclusion of implicit and nonlinear constraints as in the case of the Problem of Bolza and Hamiltonian approaches. The proposed strategy directly maximize the reaction rate term following the corresponding optimal trajectory, leading to the reactor trajectories to realizable and stable extreme values, without excessive control efforts. Numerical experiments show that the proposed control scheme is realizable keeping a satisfactory performance.

Data Availability

There is no significant data in the manuscript since most of the paper is theoretical, even though the authors declare that all the data contained in the paper are available with the corresponding author upon request.

Conflicts of Interest

The authors declare no conflicts of interest.

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