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Nonlinear Control of Diffusion-Convection-Reaction Processes

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Abstract

This work addresses the nonlinear control of a non-isothermal packed-bed reactor, modeled by two quasi-linear parabolic partial differential equations (PDEs). Initially, nonlinear Galerkin's method and the concept of approximate inertial manifold are used to derive a minimal-order ordinary differential equation (ODE) model, which accurately describes the dynamics of the process. This model is then used for the synthesis of a nonlinear finite-dimensional controller that guarantees closed-loop stability and enforces output tracking. Computer simulations are used to evaluate the performance of the controller.

1 Introduction

Transport/reaction processes arising in chemical engineering, are inherently nonlinear and are characterized by strong spatial variations due to the underlying convection and diffusion phenomena. Whenever convective mechanisms dominate over diffusive ones, these processes can be adequately described by systems of quasi-linear *hyperbolic* PDEs. These systems are characterized by spatial differential operators, whose eigenvalues cluster along vertical or nearly vertical asymptotes in the complex plane. In [4], we developed an output feedback control methodology for hyperbolic PDE systems by addressing the controller synthesis problem on the basis of the original PDE model. However, in a large number of practical applications, diffusive phenomena play a prominent role, and thus cannot be neglected. Examples include fluidized-bed and packed-bed reactors, coating processes, etc.. These processes are typically modeled by quasi-linear *parabolic* PDEs. In contrast to hyperbolic PDE systems, parabolic PDE systems involve spatial differential operators, whose eigenspectrum can be partitioned into a finite dimensional slow one and an infinite dimensional stable fast one. This fact suggests addressing the control problem on the basis of reduced-order ODE models which are able to approximately reproduce the solutions and the dynamic behavior of the original PDE model.

Motivated by the above, control methods for linear/quasi-linear parabolic PDEs utilize eigenfunction expansion techniques to obtain an approximate ODE representation of the original PDE system, which is then used for controller design purposes [1, 10, 3]. In this approach, the solution of the system is initially expanded as the sum of an infinite series of the eigenfunctions of the parabolic differential operator with time-varying coefficients. This expansion is used to derive an infinite set of ODEs for the coefficients of the expansion. Then, a finite dimensional ODE model is derived by discarding an infinite set of equations and is used for the design of finite-dimensional controllers. Finally, standard results from center manifold theory for PDE systems are employed to derive conditions for the asymptotic stability of the closed-loop system. Although this approach has been very useful in designing control systems for parabolic PDEs, it may require keeping a large number of modes to derive an ODE model that yields the desired degree of approximation, leading to high dimensionality of the resulting controllers [8]. Furthermore, this approach does not provide any information about the discrepancy between the solutions of the PDE model and the reduced-order ODE model in finite time, which is essential for characterizing the transient performance of the closed-loop system.

In [5], we presented a general framework for the synthesis of output feedback controllers for systems of quasi-linear parabolic PDEs that guarantee closed-loop stability and enforce output tracking, on the basis of *minimal-order* ODE models that accurately reproduce the spatio-temporal behavior of the PDE model. The minimal-order ODE models are derived via the construction of an approximate inertial manifold for the original PDE system, and the closed-loop system is analyzed using singular perturbation theory to establish that the requested stability and performance objectives are enforced in the closed-loop system for all times. In this paper, we illustrate the application of this control methodology to a representative diffusion-convection-reaction process, a nonisothermal packed-bed reactor. We will begin with a brief summary of the control methodology proposed in [5] and will continue with the presentation of the application.

2 Summary of control methodology

We consider processes modeled by quasi-linear parabolic PDEs, for which the manipulated input and the controlled output are distributed in space, and which have the following state-space representation:

$$
\begin{aligned}
\frac{\partial x}{\partial t} &= Lx + wb(z)u + f(x) \\
y(t) &= \int_{\Omega} c(z)kx dz \\
Ax(z,t) + B\frac{\partial x}{\partial z}(z,t) &= R(t), \; on \; \Gamma
\end{aligned}
\tag{1}
$$

where $x(z,t) \in \mathcal{H}[\Omega, \mathbb{R}^n]$, with $\mathcal{H}$ being the infinite dimensional Hilbert space of n-dimensional square integrable vector functions defined on the domain Ω, t is the time, $z = [z_1 \; z_2 \; z_3]^T$ denotes the vector of spatial variables, Γ denotes the boundary of the spatial domain Ω, $u \in \mathbb{R}$ denotes the manipulated input, $y \in \mathbb{R}$ denotes the output to be controlled, L is a linear $n \times n$ diagonal spatial differential operator of the form $L = diag\{L_i\}$, which involves first- and second-order spatial derivatives, $f(x)$ is a sufficiently smooth vector function, $b(z)$ is a smooth function which determines how the control action is distributed in space, $c(z)$ is a smooth function which depends on the desired performance specifications, w, k are constant vectors, A, B are constant matrices, and $R(t)$ is a column vector. Throughout the paper, we will use the order of magnitude notation $O(\epsilon)$. In particular, $\delta(\epsilon) = O(\epsilon)$ if there exist positive constants k and c such that: $|\delta(\epsilon)| \leq k|\epsilon|$, $\forall \; |\epsilon| < c$.

The developed framework for the synthesis of finite-dimensional output feedback controllers for systems of the form of Eq.1 entails the following steps:

- Initially, nonlinear Galerkin's method is employed to transform the model of Eq.1 into an interconnection of a finite-dimensional (possibly unstable) system with an infinite dimensional stable system. To this end, two appropriate sets of orthogonal basis functions, which completely span the space $\mathcal{H}$, are selected and used to derive a two-time-scale system, modeled within the mathematical framework of singular perturbations, whose slow subsystem is of dimension equal to the number of slow modes of the system operator L, and the fast subsystem is infinite dimensional and stable.
- Then, singular perturbation methods are employed to decompose the resulting two-time-scale system into two separate models which describe the evolution of the original system in the fast and slow time-scale, and derive a *minimal-order* slow subsystem which yields approximate solutions of desired accuracy. Given the fact that the fast subsystem is exponentially stable, a finite dimensional nonlinear output feedback controller is synthesized on the basis of the minimal-order slow subsystem, through combination of a novel iterative procedure developed in [5] and geometric nonlinear control methods (e.g. [6]), to enforce output tracking and guarantee exponential stability of the closed-loop slow subsystem.
- Finally, the resulting infinite-dimensional closed-loop system (PDE model and controller) is analyzed utilizing singular perturbation theory to derive a lower bound on the degree of separation of the slow versus the fast modes that guarantees the exponential stability of the closed-loop system and that the output satisfies a relation of the form:

$$y(t) = y^s(t) + O(\epsilon) \; , \; t > 0 \tag{2}$$

  with $y^s(t)$ being the output of the closed-loop slow subsystem and ϵ is a small positive parameter which depends on the degree of approximation of the original parabolic PDE model from the slow system and is chosen to meet certain performance specifications.

3 Control of a packed-bed reactor

3.1 Process description and analysis

We consider a non-isothermal packed-bed reactor, where an elementary endothermic reaction of the form $A \rightarrow B$ takes place. Under standard modeling assumptions, the dynamic model of the process expressed in dimensionless variables takes the form [10, 3]:

$$\begin{aligned}\frac{\partial x_1}{\partial t} &= -\frac{\partial x_1}{\partial z} + \frac{1}{Pe_T}\frac{\partial^2 x_1}{\partial z^2} - B_T B_C exp^{\gamma\frac{x_1}{1+x_1}} x_2 + \beta_T(u - x_1)\\ \frac{\partial x_2}{\partial t} &= -\frac{\partial x_2}{\partial z} + \frac{1}{Pe_C}\frac{\partial^2 x_2}{\partial z^2} - B_C exp^{\gamma\frac{x_1}{1+x_1}} x_2\end{aligned} \tag{3}$$

subject to the boundary conditions:

$$z = 0, \quad Pe_T x_1 = \frac{\partial x_1}{\partial z}, \quad Pe_C(x_2 - 1) = \frac{\partial x_2}{\partial z}; \qquad z = 1, \quad \frac{\partial x_1}{\partial z} = \frac{\partial x_2}{\partial z} = 0 \tag{4}$$

where x_1, x_2 denote dimensionless temperature and concentration in the reactor, Pe_T, Pe_C are the heat and mass Peclet numbers, B_T, B_C denote a dimensionless heat of reaction and a dimensionless pre-exponential factor, γ is a dimensionless activation energy, β_T is a dimensionless heat transfer coefficient, and u is a dimensionless jacket temperature which is assumed to be spatially uniform. The control objective is to control the temperature profile along the length of the reactor, i.e. the controlled output is of the form $y(t) = \int_0^1 x_1 dz$. The following typical values for the process parameters were used in our calculations:

$$Pe_T = 5.0, \;\; Pe_C = 5.0, \;\; B_C = 0.00001, \;\; B_T = 1.0, \;\; \beta_T = 15.62, \;\; \gamma = 22.14 \tag{5}$$

It was verified that the above process parameters correspond to a stable steady-state for the open-loop system. The process model of Eq.3 is in the form of Eq.1 with

$$L = \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{Pe_T}\frac{\partial^2 x_1}{\partial z^2} - \frac{\partial x_1}{\partial z} & 0 \\ 0 & \frac{1}{Pe_C}\frac{\partial^2 x_2}{\partial z^2} - \frac{\partial x_2}{\partial z} \end{bmatrix} \tag{6}$$

The solution of the eigenvalue problem for the above spatial differential operator subject to the boundary conditions of Eq.4 can be obtained utilizing standard techniques from linear operator theory (see for example [9, 10]) and is of the form:

$$\begin{aligned}\lambda_{ij} &= \frac{\bar{a}_{ij}^2}{Pe} + \frac{Pe}{4}, \quad i = 1,2, \;\; j = 1, \ldots, \infty\\ \phi_{ij}(z) &= B_{ij} e^{Pe\frac{z}{2}}(cos(\bar{a}_{ij} z) + \frac{Pe}{2\bar{a}_{ij}} sin(\bar{a}_{ij} z)), \quad i = 1,2, \;\; j = 1, \ldots, \infty\\ \bar{\phi}_{ij}(z) &= e^{-Pez}\phi_{ij}(z), \quad i = 1,2, \;\; j = 1, \ldots, \infty\end{aligned} \tag{7}$$

where $Pe = Pe_T = Pe_C$, and $\lambda_{ij}, \phi_{ij}, \bar{\phi}_{ij}$, denote the eigenvalues, eigenfunctions and adjoint eigenfunctions of L_i, respectively. $\bar{a}_{ij}, B_{ij}$ can be calculated from the following formulas:

$$\begin{aligned}tan(\bar{a}_{ij}) &= \frac{Pe\bar{a}_{ij}}{\bar{a}_{ij}^2 - (\frac{Pe}{2})^2}, \quad i = 1,2, \;\; j = 1, \ldots, \infty\\ B_{ij} &= \left\{\int_0^1 \left(cos(\bar{a}_{ij} z) + \frac{Pe}{2\bar{a}_{ij}} sin(\bar{a}_{ij} z)\right)^2 dz\right\}^{-\frac{1}{2}}, \quad i = 1,2, \;\; j = 1, \ldots, \infty\end{aligned} \tag{8}$$

A direct computation of the first five eigenvalues of L yields $\lambda_{11} = \lambda_{21} = 1.94, \lambda_{12} = \lambda_{22} = 4.80, \lambda_{13} = \lambda_{23} = 10.42, \lambda_{14} = \lambda_{24} = 20.93$, and $\lambda_{15} = \lambda_{25} = 34.78$. These values indicate that the eigenspectrum of L exhibits a two-time-scale property and suggest considering the first two eigenmodes of each PDE as the slow ones and the remaining infinite eigenmodes as the fast ones.

3.2 Construction of minimal-order ODE models

We will initially utilize nonlinear Galerkin's method [10, 2] to transform the PDE model of Eq.3 into an equivalent set of infinite ODEs. The solution of the state x_i of the system of Eq.3 can be represented in terms of the eigenfunctions ϕ_{ij}, in the following way:

$$x_i(z,t) = \sum_{j=1}^{\infty} a_{ij}(t)\phi_{ij}(z) \tag{9}$$

where $a_{ij}(t)$ are time-varying coefficients. Defining the orthogonal projection operators P_{s_i} and P_{f_i}, $i = 1,2$, as:

$$P_{s_i}x_i(z,t) = \sum_{j=1}^{2} a_{ij}(t)\phi_{ij}(z), \quad P_{f_i}x_i(z,t) = \sum_{j=3}^{\infty} a_{ij}(t)\phi_{ij}(z) \tag{10}$$

the state of the system of Eq.3 can be decomposed as

$$x = x_s + x_f = P_s x + P_f x \tag{11}$$

where $P_s x = [P_{s_1}^T x_1 \; P_{s_2}^T x_2]^T$, $P_f x = [P_{f_1}^T x_1 \; P_{f_2}^T x_2]^T$. Substituting Eq.11 into Eq.3 and applying the projection operators P_s and P_f, a dynamical system consisting of an infinite set of ODEs is obtained, which after grouping the first 4 equations corresponding to the slow eigenmodes, can be compactly written in the following form:

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + w b_s u + f_s(x_s, x_f) \\ \frac{\partial x_f}{\partial t} &= A_f x_f + w b_f u + f_f(x_s, x_f) \\ y &= Ckx_s + Ckx_f \end{aligned} \tag{12}$$

where $A_s = P_s A P_s$, $b_s = P_s b$, $f_s = P_s f$, $A_f = P_f A P_f$, $b_f = P_f b$, $f_f = P_f f$. In the above system, A_s is a 4×4 diagonal matrix of the form $A_s = diag\{\lambda_{11}, \lambda_{12}, \lambda_{21}, \lambda_{22}\}$, f_s and f_f are smooth vector functions, and A_f is an exponentially stable differential operator whose smallest eigenvalue is $\lambda_{13} = \lambda_{23}$. Defining $\epsilon_p = \dfrac{\lambda_{11}}{\lambda_{13}} = \dfrac{\lambda_{21}}{\lambda_{23}}$ and multiplying the x_f-subsystem of Eq.12 by ϵ_p, the system of Eq.12 can be written in the singularly perturbed form:

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + w b_s u + f_s(x_s, x_f) \\ \epsilon_p \frac{\partial x_f}{\partial t} &= A_f^{\epsilon} x_f + \epsilon_p w b_f u + \epsilon_p f_f(x_s, x_f) \\ y &= Ckx_s + Ckx_f \end{aligned} \tag{13}$$

where A_f^{ϵ} is an exponentially stable differential operator, whose smaller eigenvalue is identical to the smaller eigenvalue of the matrix A_s. Owing to its two-time-scale property, the trajectories of the system of Eq.13 starting from arbitrary initial conditions, converge to a finite-dimensional stable inertial manifold M [7], after a short initial transient. On the inertial manifold, the solution of the PDE system of Eq.3 is exactly described by the solutions of the finite-dimensional slow system (called inertial form):

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + w b_s u + f_s(x_s, \Sigma(x_s, u, \epsilon_p)) \\ y^s &= Ckx_s + Ck\Sigma(x_s, u, \epsilon_p) \end{aligned} \tag{14}$$

and the manifold equation $x_f = \Sigma(x_s, u, \epsilon_p)$. In order to derive the explicit form of the exact slow system, we need to compute the analytic form of $\Sigma(x_s, u, \epsilon_p)$. However, this computation cannot be performed analytically due to the complexity of the process under consideration. Instead, we will compute approximations of the exact slow system of arbitrary accuracy by constructing approximations of $\Sigma(x_s, u, \epsilon_p)$ (called approximate inertial manifolds). In [5], we developed a novel procedure for the construction of approximations of $\Sigma(x_s, u, \epsilon_p)$ of arbitrary accuracy using singular perturbation theory (see also [2] for an alternative approach for the construction of approximate inertial manifolds). This procedure involves expansion of $\Sigma(x_s, u, \epsilon_p)$ and u in a power series in ϵ_p:

$$\begin{aligned} u(x_s, \epsilon_p) &= u_0(x_s, \epsilon_p) + \epsilon_p u_1(x_s, \epsilon_p) + \cdots + \epsilon_p^k u_k(x_s, \epsilon_p) + O(\epsilon_p^{k+1}) \\ \Sigma(x_s, u, \epsilon_p) &= \Sigma^0(x_s, u) + \epsilon_p \Sigma^1(x_s, u) + \cdots + \epsilon_p^k \Sigma^k(x_s, u) + O(\epsilon_p^{k+1}) \end{aligned} \tag{15}$$

where u_k, Σ^k are smooth functions, followed by the substitution of the resulting expressions into the equation:

$$\dot{x}_f = \frac{\partial \Sigma}{\partial x_s}\dot{x}_s + \frac{\partial \Sigma}{\partial u}\dot{u} \tag{16}$$

(which was obtained by differentiating in time the manifold equation $x_f = \Sigma(x_s, u, \epsilon_p)$), and equation of terms of the same power in ϵ_p. Following this procedure, the $O(\epsilon_p)$ approximation of $\Sigma(x_s, u, \epsilon_p)$ is $\Sigma^0(x_s, u) = 0$ and the $O(\epsilon_p)$ approximation of the exact slow system takes the form:

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + w b_s u_0 + f_s(x_s, 0) \\ y^s &= Ckx_s \end{aligned} \tag{17}$$

Furthermore, the $O(\epsilon_p^2)$ approximation of $\Sigma(x_s,u,\epsilon_p)$ has the form:

$$\Sigma(x_s,u,\epsilon_p)=\Sigma^0(x_s,u_0)+\epsilon_p\Sigma^1(x_s,u)+O(\epsilon_p^2)=0+\epsilon_p(A_f^\epsilon)^{-1}[-wb_fu_0-f_f(x_s,0)]+O(\epsilon_p^2) \tag{18}$$

and the corresponding $O(\epsilon_p^2)$ approximation of the exact slow system is given by:

$$\begin{aligned}\frac{dx_s}{dt} &= A_sx_s+wb_su_0+\epsilon_pwb_su_1+f_s(x_s,\epsilon_p(A_f^\epsilon)^{-1}[-wb_fu_0-f_f(x_s,0)])\\ y_s &= Ckx_s+\epsilon_pCk(A_f^\epsilon)^{-1}[-wb_fu_0-f_f(x_s,0)]\end{aligned} \tag{19}$$

3.3 Controller synthesis-Simulations

The ODE model of Eq.19 was used for the synthesis of a nonlinear finite-dimensional controller consisting of a static state feedback law u of the form:

$$u = u_0+\epsilon_pu_1=p_0(x_s)+Q_0(x_s)v+\epsilon_p[p_1(x_s,\epsilon_p)+Q_1(x_s,\epsilon_p)v] \tag{20}$$

where p_0,Q_0,p_1,Q_1 are smooth functions and v is the set point, coupled with an open-loop observer of the form of Eq.19 (this is possible because the open-loop process and thus the model of Eq.19 are exponentially stable). The synthesis of the static control law was performed following an iterative procedure which was proposed in [5]. In particular, the leading term of the expansion, u_0, was synthesized employing geometric control methods (e.g., [6]) on the basis of the $O(\epsilon_p)$ approximation of the exact slow system (Eq.17), followed by the synthesis of the term u_1 on the basis of the $O(\epsilon_p^2)$ ($O(0.036)$) approximation of the exact slow system (Eq.19). The $O(\epsilon_p^2)$ approximation of $\Sigma(x_s,u,\epsilon_p)$ was constructed by retaining the first three of the fast modes for each PDE, and discarding the remaining infinite ones (this is because the use of more than three fast modes provides negligible improvement in the accuracy of the $O(\epsilon_p^2)$ approximation of the fourth-order model). Furthermore, the ODE system of Eq.14, with the $O(\epsilon_p)$ and $O(\epsilon_p^2)$ approximations of $\Sigma(x_s,u,\epsilon_p)$ was found to be minimum-phase (i.e., its zero dynamics is exponentially stable), which implies that the controller guarantees exponential stability of the closed-loop slow system. Finally, it was also established that the value of $\epsilon_p = 0.19$ ensures that the controller exponentially stabilizes the closed-loop parabolic PDE system as well.

Simulation runs were performed to illustrate the advantages obtained by using higher-order approximations of $\Sigma(x_s,u,\epsilon_p)$ in the construction of the slow subsystem of Eq.14 and evaluate the output tracking capabilities of the proposed control methodology. In particular, we compared the performance of the controller synthesized following the above procedure with that of a controller consisting of the static control law $u=u_0$ coupled with an open-loop observer of the form of Eq.17 ($O(\epsilon_p)$ approximation). The results of the simulation study are given in Figure 1. The left figures show the output and manipulated input profiles for an 8.0% decrease in the value of the set-point (the new set-point value is $v=1.11$). It is clear that the controller synthesized on the basis of the model which uses an $O(\epsilon_p^2)$ approximation for $\Sigma(x_s,u,\epsilon_p)$ provides an excellent performance driving the output (solid line) very close to the new set-point (note that as expected, $lim_{t\to\infty}|y-v|=O(\epsilon_p^2)$). On the other hand, the controller synthesized on the model of Eq.17 drives the output (dotted line) to a neighborhood of the set-point (note that $lim_{t\to\infty}|y-v|=O(\epsilon_p)$) leading to significant offset (compare with set-point value). The right figure displays the evolution of the dimensionless temperature of the reactor for the case of using an $O(\epsilon_p^2)$ approximation for $\Sigma(x_s,u,\epsilon_p)$. The controller achieves excellent performance, regulating the temperature at each point of the reactor to a new steady-state value, which is close to 8% lower than the one of the original steady-state. Finally, it was also verified through simulations (not shown here due to space limitations) that: *i*) the closed-loop output profile obtained by using a fourth-order model with an $O(\epsilon_p^2)$ approximation for $\Sigma(x_s,u,\epsilon_p)$ is comparable to the one achieved by using a tenth-order model with an $O(\epsilon_p)$ approximation for $\Sigma(x_s,u,\epsilon_p)$, and *ii*) the use of higher-order approximations for $\Sigma(x_s,u,\epsilon_p)$ and $u(x_s,\epsilon_p)$ (i.e. $O(\epsilon_p^3)$) in the construction of the fourth-order model provides minimal improvement. From the results of the simulation study, it is evident that the methodology proposed in [5] is a powerful tool for the synthesis of *minimal-order* controllers which yield a desired closed-loop performance for diffusion-convection-reaction processes.

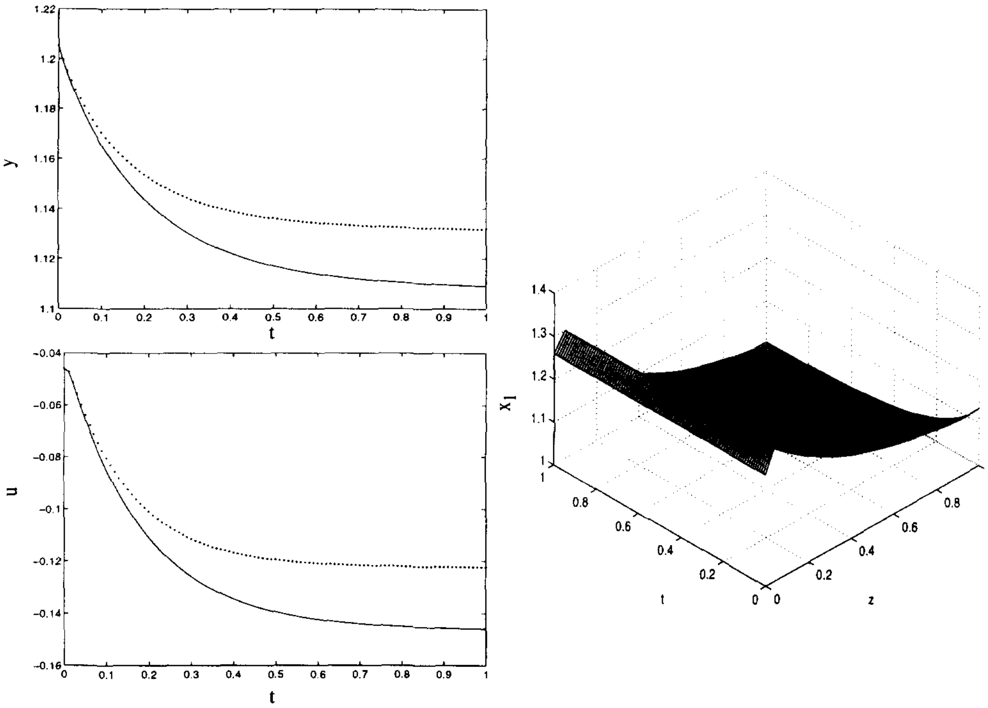

Figure 1: *Left figures.* Comparison of output (top figure) and manipulated input (bottom figure) profiles of the closed-loop system, for an 8% decrease in the set point. The solid lines correspond to a controller based on the model of Eq.14 with an $O(\epsilon_p)$ approximation for Σ, while the dotted lines correspond to a controller based on the model of Eq.14 with an $O(\epsilon_p^2)$ approximation for Σ. *Right figure.* Profile of evolution of reactor temperature, for an 8% decrease in the set point ($O(\epsilon_p^2)$ approximation for Σ).

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