Pergamon

Chemical Engineering Science, Vol. 53, No. 8, pp. 1491–1504, 1998

Printed in Great Britain

PII: S0009-2509(98)00006-2

0009-2509/98 $19.00 + 0.00

Singular perturbation modeling of nonlinear processes with nonexplicit time-scale multiplicity

Aditya Kumar, Panagiotis D. Christofides* and Prodromos Daoutidis†

Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

(Received 7 October 1996; accepted 18 April 1997)

Abstract—In this article, a modeling framework is proposed for two-time-scale chemical processes modeled by nonlinear ordinary differential equations (ODEs) with large parameters of the form $1/\varepsilon$, to obtain a standard singularly perturbed representation where the slow and fast variables are explicitly separated. Initially, a result is derived that provides necessary and sufficient conditions for the existence and the explicit form of an ε-independent coordinate change that transforms the two-time-scale process into a standard singularly perturbed form. Whenever these conditions are not satisfied, it is established that an ε-dependent coordinate change, *singular* at $\varepsilon = 0$, has to be employed to obtain a standard singularly perturbed representation of the original two-time-scale process, and the construction of such a transformation is addressed. The application of the proposed framework in deriving standard singularly perturbed representations and its significance in the synthesis of well-conditioned controllers is demonstrated through chemical reactor applications.

Keywords: Singularly perturbed systems; high-index DAE systems; slightly nonminimum-phase processes; nonlinear control.

1. INTRODUCTION

Chemical processes are inherently nonlinear and often involve physical and chemical phenomena occurring in different time scales. Typical multiple-time-scale processes include catalytic reactors, fluidized catalytic crackers, chemical vapor deposition reactors, and multi-phase reactors, where the time-scale multiplicity arises due to the presence of large thermal capacitances, significantly different residence times, multiple fast and slow reactions, and fast mass/heat transfer. It is well established that a direct application of standard inversion-based control algorithms to multiple-time-scale processes, ignoring the presence of time-scale multiplicity, may lead to controller illconditioning (i.e. the controller generates very large control actions in the presence of small measurement/modeling errors) and/or closed-loop instability (Kokotovic *et al.*, 1986; Christofides and Daoutidis, 1996b).

Singular perturbation theory has proven to be a natural framework for modeling, stability analysis and synthesis of well-conditioned controllers for two-time-scale processes (Kokotovic *et al.*, 1986). The main requirement for the application of singular perturbation methods to two-time-scale processes is that the process has to be modeled in the *standard* singularly perturbed form, where the separation of fast and slow variables is explicit due to the presence of a small parameter ε (called singular perturbation parameter) that multiplies the time derivative of the vector of fast variables. In many two-time-scale processes, there is *a priori* knowledge of the fast and slow variables. This allows modeling such processes, through an appropriate definition of ε, directly in a standard singularly perturbed form where the separation of fast and slow variables is consistent with the process dynamics. For example, in a catalytic reactor where the catalytic phase typically has a large heat capacitance, the fast and slow variables are associated with the homogeneous and catalytic phases, respectively. Thus, choosing ε as the reciprocal of the large heat capacitance of the catalytic phase, the process model can be directly written in a standard singularly perturbed form (Chang and Aluko, 1984; Christofides and Daoutidis,

* Present address: Department of Chemical Engineering, University of California, Los Angeles CA 90024, U.S.A.

† Corresponding author. Tel.: (612) 625-8818; fax: (612) 626 7246; e-mail: daoutidi@cems.umn.edu.

1996a). Similarly, in a fluidized catalytic cracking process where the residence time in the reactor is much smaller than that in the regenerator, the fast and slow variables are associated with the reactor and the regenerator, respectively. Thus, defining ε as the ratio of the residence time in the reactor over the residence time in the regenerator, a standard form representation of the process can be directly obtained (Denn, 1986).

On the other hand, there is a wide range of applications that exhibit time-scale multiplicity, but for which the slow and fast dynamics cannot be associated with distinct process variables. Owing to this lack of *a priori* knowledge of the fast and slow variables, such processes cannot be directly modeled in the standard singularly perturbed form. For such systems, the derivation of a standard singularly perturbed representation requires the use of a coordinate change. The construction of such a coordinate change for linear two-time-scale systems is addressed using modal analysis (see, for example Georgakis, 1977). However, for nonlinear systems, modal analysis is not applicable and in general, a nonlinear coordinate change is required. An early work on two-time-scale systems modeled by nonlinear ODEs with a small parameter ε focused on studying their geometric properties to obtain a coordinate-free characterization of the time-scale multiplicity (Fenichel, 1979). This characterization was subsequently used to derive necessary and sufficient geometric conditions for the existence of an ε-independent change of coordinates that yields a standard singularly perturbed representation (Marino and Kokotovic, 1988). A specific ε-independent coordinate change was proposed for a class of reaction networks with fast and slow reactions in Breusegem and Bastin (1991), whereas an ε-dependent coordinate change for a class of nonlinear two-time-scale systems was also proposed in Krishnan and McClamroch (1994).

In this article, we consider a class of nonlinear ODEs with large parameters of the form $1/\varepsilon$, which arise naturally as models of two-time-scale chemical processes with nonexplicit time-scale separation. For such systems, our objective is to develop a framework for the systematic construction of nonlinear coordinate changes that yield standard singularly perturbed representations. To this end, we initially derive (i) necessary and sufficient conditions for the existence of an ε-independent coordinate change, given explicitly in terms of the modeling equations, and (ii) the precise form of such a coordinate change. For systems that do not satisfy these conditions, we establish that the ε-dependent coordinate change that has to be employed to obtain a standard singularly perturbed form, has to be necessarily singular at $\varepsilon = 0$, and thus the resulting standard form is valid in a state-space region that shrinks with ε. The construction of such an ε-dependent coordinate change is also addressed. Finally, we consider two examples of chemical processes with nonexplicit time-scale separation where standard input/output linearizing controllers designed on the basis of the process model, ignoring the time-scale multiplicity, lead to problems of ill-conditioning and instability. On the other hand, controllers designed on the standard form representations obtained through the proposed modeling framework, are well conditioned and yield excellent performance with stability. In the first example, we consider a reactor with a heating jacket where the heat transfer between the reactor and the jacket is fast compared to the reaction. For this process, we show that an ε-independent coordinate change can be used to derive a standard form representation. In the second example, we consider a chemical reactor with multiple reactions where some reactions are much faster than the others, leading to a two-time-scale behavior. For this process, an ε-dependent coordinate change has to be used to derive a standard form representation.

2. MODELS OF TWO-TIME-SCALE SYSTEMS

The majority of results on stability analysis and control of two-time-scale systems have been derived for systems modeled in the standard singularly perturbed form

$$\begin{aligned} \dot{\zeta} &= F(\zeta, \eta, u, \varepsilon) \\ \varepsilon\dot{\eta} &= G(\zeta, \eta, u, \varepsilon) \\ y_i &= h_i(\zeta, \eta), \quad i = 1, \ldots, m \end{aligned} \tag{1}$$

where $\zeta \in \mathscr{Z} \subset \mathbb{R}^{n_1}$, $\eta \in \mathscr{Y} \subset \mathbb{R}^{n_2}$ are the state variables with $\mathscr{Z}$, $\mathscr{Y}$ being open and connected sets, $u \in \mathbb{R}^m$ is the vector of manipulated inputs, y_i's are the outputs to be controlled, ε is a small positive parameter, F, G are analytic vector fields of dimensions n_1 and n_2, respectively, h_i are analytic scalar functions, and $G(\zeta, \eta, u, 0) = 0$ has k isolated real roots $\eta_i = \alpha_i(\zeta, u)$, $i = 1, \ldots, k$, i.e. the Jacobian $(\partial G(\zeta, \eta, u, 0)/\partial\eta)$ is nonsingular. Owing to the presence of the small parameter ε that multiplies the time derivative of η, the system of eq. (1) is characterized by an explicit time-scale separation with the states η being the fast ones and the states ζ being the slow ones. Although many two-time-scale chemical processes (e.g. catalytic and fluidized catalytic cracking reactors) can be directly modeled in the form of eq. (1) through appropriate definition of ε, there is a wide variety of processes that exhibit time-scale multiplicity but for which the separation of slow and fast variables is not explicit. Typical examples of such processes include those with multiple fast and slow reactions, or fast heat/mass transfer. A common feature of these processes is that their dynamic models involve large parameters of the form $1/\varepsilon$ (e.g. large reaction rate coefficients, large heat/mass transfer coefficients) and are described by systems of the form (see, for example, the processes studied in Section 4):

$$\begin{aligned} \dot{x} &= f(x) + g(x)\,u + \frac{1}{\varepsilon}\,b(x)k(x) \\ y_i &= h_i(x), \quad i = 1, \ldots, m \end{aligned} \tag{2}$$

where $x \in \mathcal{X} \subset \mathbb{R}^n$ is the vector of state variables, $f(x)$, $k(x)$ are analytic vector fields of dimensions n and p ($p < n$), $g(x)$, $b(x)$ are analytic matrices of dimensions $n \times m$, $n \times p$, respectively.

In this article, we consider systems of the form of eq. (2) for which the matrix $b(x)$ and the Jacobian $(\partial k(x)/\partial x)$ have full column and row rank, respectively. The condition on the rank of $b(x)$ is not restrictive. For, if rank $b(x) = \bar{p} < p$, then there always exists a nonsingular $p \times p$ matrix $E(x)$ such that

$$b(x)\, k(x) = b(x)\, E(x)\, E(x)^{-1} k(x) = [\bar{b}(x)\ \ 0]\, \bar{k}(x)$$

where $\bar{b}(x)$ has full column rank $\bar{p}$. Thus, discarding the $(p - \bar{p})$ columns that are zero and the corresponding last $(p - \bar{p})$ components of $\bar{k}(x)$, a system in the form of eq. (2) is obtained where the new matrix $\bar{b}(x)$ has full column rank. The condition on the rank of $(\partial k(x)/\partial x)$ is required to ensure that in the limit $\varepsilon = 0$, the DAE system that describes the slow dynamics of eq. (2) (see the next section) has a finite index and a well-defined solution, and it is satisfied in typical chemical process applications (see the reactor examples studied in Section 4).

Throughout this article, we will use the order of magnitude notation $O(\varepsilon)$, where $\delta(\varepsilon) = O(\varepsilon)$ if there exist positive constants k and c such that: $|\delta(\varepsilon)| \leq k|\varepsilon|$, $\forall\ |\varepsilon| < c$. Moreover, $L_b k(x)$ will be used to denote the matrix with the (i, j)th component given by the standard Lie derivative $L_{b_j} k_i(x)$, where b_j is the jth column of $b(x)$ and k_i is the ith component of $k(x)$ (see the appendix for the definition of Lie derivative).

3. DERIVATION OF STANDARD SINGULARLY PERTURBED FORM

In this section, the objective is to study the problem of constructing coordinate changes that yield standard singularly perturbed representations of the system in eq. (2). To this end, we perform a two-time-scale decomposition on the system of eq. (2) to derive separate representations of its slow and fast dynamics in the appropriate time scales, and obtain some insight on the variables that will be used as part of the coordinate change. More specifically, in the slow time-scale t, multiplying eq. (2) by ε and considering the limit $\varepsilon \to 0$, the following constraints are obtained:

$$k_i(x) = 0, \quad i = 1, \ldots, p \tag{3}$$

where $k_i(x)$ denotes the ith component of $k(x)$. These constraints must be satisfied in the slow subsystem. Defining $\lim_{\varepsilon \to 0} k_i(x)/\varepsilon = z_i$ and taking the limit $\varepsilon \to 0$ in the system of eq. (2), the following system is obtained:

$$\begin{aligned} \dot{x} &= f(x) + g(x)\, u + b(x) z \\ 0 &= k(x) \end{aligned} \tag{4}$$

which describes the slow dynamics of eq. (2). Note that the above system is a differential algebraic equation (DAE) system where x is the vector of differential variables and $z \in \mathbb{R}^p$ is the vector of algebraic variables. For the DAE system of eq. (4), the index ν_d is defined as the minimum number of times the algebraic equations $k(x) = 0$ have to be differentiated to obtain explicit differential equations for z (Brenan *et al.*, 1996). Clearly, the DAE system in eq. (4) has a high index ($\nu_d > 1$), and thus it is characterized by the presence of algebraic constraints in the differential variables x. In particular, the algebraic equations in eq. (4) already denote p such constraints, and depending on the index, additional constraints may also be present. These constraints specify the dimension of the subspace in $\mathcal{X}$ where the slow dynamics of the two-time-scale system of eq. (2) evolves.

On the other hand, introducing the fast time-scale $\tau = t/\varepsilon$ and considering the limit $\varepsilon \to 0$ in the system of eq. (2), the following representation of the fast dynamics of eq. (2) is obtained:

$$\frac{dx}{d\tau} = b(x)k(x). \tag{5}$$

From the above system, it is clear that in the fast time-scale τ, the algebraic constraints of eq. (3) are not satisfied i.e. $k(x) \neq 0$. The fact that $k_i(x)$, $i = 1, \ldots, p$ are identically zero in the slow system of eq. (4) in the slow time-scale t, while they are nonzero for the system of eq. (5) in the fast time-scale τ, implies that they can be used in the definition of the fast variables in the coordinate change.

Theorem 1 provides necessary and sufficient conditions for the existence of an ε-independent coordinate change that transforms the two-time-scale system of eq. (2) into a standard form (a proof is given in the appendix).

Theorem 1: *Consider the system of eq.* (2), *for which the slow dynamics is described by the DAE system of eq.* (4). *The system of eq.* (2) *can be transformed into a two-time-scale singularly perturbed system in standard form through an ε-independent nonlinear coordinate change, if and only if*

(i) *the* $\mathrm{p} \times \mathrm{p}$ *matrix* $\mathrm{L_b k(x)}$ *is nonsingular on* $\mathcal{X}$, *and*
(ii) *the* p*-dimensional distribution* $\mathrm{B(x) = span\ \{b_1(x), \ldots, b_p(x)\}}$ *is involutive (see the appendix for the definition of involutivity).*

If these conditions hold, then under the coordinate change

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x) = \begin{bmatrix} \phi(x) \\ k(x) \end{bmatrix} \tag{6}$$

where $\zeta \in \mathbb{R}^{n-p}$, $\eta \in \mathbb{R}^p$ *and* $\phi(x)$ *is a vector field of dimension* $(n - p)$ *with components* $\phi_i(x)$ *such that* $L_{b_j}\phi_i(x) = 0$, $\forall$ i, j, *the system of eq.* (2) *takes the following standard singularly perturbed form:*

$$\begin{aligned} \dot{\zeta} &= \tilde{f}(\zeta, \eta) + \tilde{g}(\zeta, \eta)u \\ \varepsilon\dot{\eta} &= \varepsilon\bar{f}(\zeta, \eta) + \varepsilon\bar{g}(\zeta, \eta)u + Q(\zeta, \eta)\eta \\ y_i &= h_i(\zeta, \eta), \quad i = 1, \ldots, m \end{aligned} \tag{7}$$

where $\tilde{f} = L_f\phi(x)|_{x=T^{-1}(\zeta,\eta)}$, $\bar{f} = L_f k(x)|_{x=T^{-1}(\zeta,\eta)}$, $\tilde{g} = L_g\phi(x)|_{x=T^{-1}(\zeta,\eta)}$, $\bar{g} = L_g k(x)|_{x=T^{-1}(\zeta,\eta)}$, $Q = L_b k(x)|_{x=T^{-1}(\zeta,\eta)}$ *and* $Q(\zeta, \eta)$ *is nonsingular uniformly in* $\zeta \in \mathbb{R}^{n-p}$, $\eta \in \mathbb{R}^p$.

Remark 1: Condition (i) of Theorem 1 essentially means that the corresponding DAE system in eq. (4) has an index two, which directly fixes the dimensions of the fast and slow variables to p and $n - p$, respectively. This condition is satisfied for a wide variety of DAE systems arising in chemical engineering (see, for example, the applications studied in Kumar and Daoutidis (1995) and in Section 4 of this article). Condition (ii) of the theorem ensures that the $(n - p)$-dimensional slow ζ-subsystem can be made independent of the singular term $(1/\varepsilon)$, thereby yielding the system of eq. (7) in the standard singularly perturbed form. While condition (ii) is trivially satisfied for all linear systems and for nonlinear systems with $p = 1$, it is not satisfied in general for nonlinear systems with $p > 1$.

Remark 2: In Marino and Kokotovic (1988), two-time-scale systems of the general form

$$\frac{dx}{d\tau} = f(x, u, \varepsilon) \tag{8}$$

were considered in the fast time-scale τ. For these systems necessary and sufficient geometric conditions were derived for the existence of an ε-independent coordinate change of the form: $\zeta = \phi_s(x)$, $\eta = \phi_f(x)$ that transforms them into an equivalent system in the standard singularly perturbed form of eq. (1). Owing to the generality of the form in eq. (8), these geometric conditions ((i) the existence of an equilibrium manifold, (ii) the existence of a family of conservation manifolds, and (iii) the transversality of the equilibrium and conservation manifolds) were expressed in an abstract coordinate-free setting. On the other hand, conditions (i) and (ii) of Theorem 1 are readily verifiable, and they comprise an *explicit* coordinate-dependent form of the geometric conditions in Marino and Kokotovic (1988) for two-time-scale systems with the specific structure of eq. (2). The latter point can be verified for the system of eq. (2) in the fast time-scale:

$$\frac{dx}{d\tau} = \varepsilon f(x) + \varepsilon g(x)u + b(x)k(x) \tag{9}$$

where in the limiting case $\varepsilon \to 0$, the constraints $k(x) = 0$ specify the $(n - p)$-dimensional equilibrium manifold $E^u = \{x \in \mathcal{X}: k(x) = 0\}$, and $C = \{x \in \mathcal{X}: \phi(x) = c \in R^{(n-p)}\}$ denotes the family of p-dimensional conservation manifolds that are transversal to the equilibrium manifold E^u.

Motivated by the fact that the involutivity condition (ii) may be easily violated in general nonlinear systems with $p > 1$, we will now consider systems of eq. (2) for which the distribution $B(x)$ is not involutive. For such systems, we provide a result in the following theorem which states the implications of the lack of involutivity of $B(x)$ on the two-time-scale property and the structure of the coordinate change required for obtaining a standard singularly perturbed representation (for a proof, see the appendix).

Theorem 2: *Consider the system of eq.* (2) *for which the* $p \times p$ *matrix* $L_b k(x)$ *is nonsingular on* $\mathcal{X}$ *and the distribution* $B(x)$ *is not involutive. Then,*

(i) *this system exhibits two-time-scale behavior in a region* $\mathcal{M}(\varepsilon) \subset \mathcal{X}$, *where* $k_i(x) = O(\varepsilon)$ *for some* $i \in [1, p]$, *and*

(ii) *an* ε*-dependent coordinate change, singular at* $\varepsilon = 0$, *is necessary to obtain a standard form representation of this system.*

Remark 3: The results of Theorems 1 and 2 demonstrate the connection between the involutivity of $B(x)$ and the size of the state-space region in which the system of eq. (2) exhibits the two-time-scale property as well as the nature of the coordinate transformation required. Specifically, if $B(x)$ is involutive, the size of this state-space region is independent of ε, whereas if $B(x)$ is not involutive, the size of this state-space region depends explicitly on ε in a singular fashion and it shrinks as $\varepsilon \to 0$ (the reader may refer to Kumar *et al.* (1996) for details and an illustrative example).

An ε-dependent coordinate change that is singular at $\varepsilon = 0$ and can be used to derive a standard singularly perturbed representation of the system in eq. (2), can be obtained following Krishnan and McClamroch (1994) and is of the form:

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x, \varepsilon) = \begin{bmatrix} \phi(x) \\ \dfrac{k(x)}{\varepsilon} \end{bmatrix} \tag{10}$$

where $\zeta \in \mathbb{R}^{n-p}$ is the vector of slow variables and $\eta \in \mathbb{R}^p$ is the vector of fast variables. Under the coordinate change of eq. (10), the two-time-scale system of eq. (2) takes the following standard form:

$$\begin{aligned} \dot{\zeta} &= \tilde{f}(\zeta, \varepsilon\eta) + \tilde{g}(\zeta, \varepsilon\eta)u + \tilde{b}(\zeta, \varepsilon\eta)\eta \\ \varepsilon\dot{\eta} &= \bar{f}(\zeta, \varepsilon\eta) + \bar{g}(\zeta, \varepsilon\eta)u + Q(\zeta, \varepsilon\eta)\eta \\ y_i &= h_i(\zeta, \varepsilon\eta), \quad i = 1, \ldots, m \end{aligned} \tag{11}$$

where $\tilde{f} = L_f\phi(x)$, $\bar{f} = L_f k(x)$, $\tilde{g} = L_g\phi(x)$, $\bar{g} = L_g k(x)$, $Q = L_b k(x)$, $\tilde{b} = L_b\phi(x)$, evaluated at $x = T^{-1}(\zeta, \varepsilon\eta)$, and $Q(\zeta, 0)$ is nonsingular uniformly in $\zeta \in \mathbb{R}^{n-p}$.

The coordinate change of eq. (10) essentially defines the fast variables η as the constraints $k(x)$ 'stretched' by a factor $1/\varepsilon$, thereby making the ε-dependent region $\mathcal{M}(\varepsilon)$ of Theorem 2, independent of ε in the transformed coordinates (ζ, η). However, such a coordinate change may be unnecessarily restrictive in the sense that the resulting standard singularly perturbed representation of eq. (11) is valid only in a subspace region $\bar{\mathcal{M}}(\varepsilon) = \{x \in \mathcal{X}: k_i(x) = O(\varepsilon), \textit{ for all } i\}$. Motivated by this, we now propose a coordinate change that 'stretches' a minimal number of fast variables by the factor $1/\varepsilon$, thereby yielding a standard singularly

perturbed representation of the system of eq. (2) which is valid in a larger region. The result is given in the following proposition.

Proposition: *Consider the system of eq.* (2), *for which the* $p \times p$ *matrix* $L_b k(x)$ *is nonsingular on* $\mathcal{X}$ *and the distribution* $B(x)$ *is not involutive. For this system, let* $\bar{p} < p$ *be the largest integer such that, after possibly rearranging the columns of* $b(x)$ *and correspondingly the rows of* $k(x)$,

(i) *the distribution* $\bar{B}(x) = \text{span}\{b_1(x), \ldots, b_{\bar{p}}(x)\}$ *is involutive, and*
(ii) $L_{b_j} k_i(x) = 0; \quad i = \bar{p}+1, \ldots, p, \quad j = 1, \ldots, \bar{p}.$

Then, under the coordinate change,

$$\begin{bmatrix} \zeta \\ \eta_1 \\ \eta_2 \end{bmatrix} = T(x, \varepsilon) = \begin{bmatrix} \phi(x) \\ k^1(x) \\ \hline \dfrac{k^2(x)}{\varepsilon} \end{bmatrix} \tag{12}$$

where $\zeta \in \mathbb{R}^{n-p}, \eta_1 \in \mathbb{R}^{p}, \eta_2 \in \mathbb{R}^{p-\bar{p}}$, $k^1(x), k^2(x)$ *are vector fields comprised of the first* $\bar{p}$ *and last* $p - \bar{p}$ *components of* $k(x)$, *respectively, and* $\phi(x)$ *is a vector field of dimension* $(n - p)$ *with components* $\phi_i(x)$ *such that* $L_{b_j}\phi_i(x) \equiv 0, j = 1, \ldots, \bar{p}, \ \forall i$, *the system of eq.* (2) *takes the following standard singularly perturbed form:*

$$\begin{aligned}
\dot{\zeta} &= \bar{f}(\zeta, \eta_1, \varepsilon\eta_2) + \bar{g}(\zeta, \eta_1, \varepsilon\eta_2)u + \bar{b}(\zeta, \eta_1, \varepsilon\eta_2)\eta_2 \\
\varepsilon\dot{\eta}_1 &= \varepsilon\bar{f}_1(\zeta, \eta_1, \varepsilon\eta_2) + \varepsilon\bar{g}_1(\zeta, \eta_1, \varepsilon\eta_2)u \\
&\quad + Q_{11}(\zeta, \eta_1, \varepsilon\eta_2)\eta_1 + \varepsilon Q_{12}(\zeta, \eta_1, \varepsilon\eta_2)\eta_2 \\
\varepsilon\dot{\eta}_2 &= \bar{f}_2(\zeta, \eta_1, \varepsilon\eta_2) + \bar{g}_2(\zeta, \eta_1, \varepsilon\eta_2)u \\
&\quad + Q_{22}(\zeta, \eta_1, \varepsilon\eta_2)\eta_2 \\
y_i &= h_i(\zeta, \eta_1, \varepsilon\eta_2), \quad i = 1, \ldots, m
\end{aligned} \tag{13}$$

where $\bar{f} = L_f\phi(x)$, $\bar{g} = L_g\phi(x)$, $\bar{b} = L_{b^2}\phi(x)$, $\bar{f}_i = L_f k^i(x)$, $\bar{g}_i = L_g k^i(x)$, $Q_{11} = L_{b^1}k^1(x)$, $Q_{12} = L_{b^2}k^1(x)$, $Q_{22} = L_{b^2}k^2(x)$ *evaluated at* $x = T^{-1}(\zeta, \eta_1, \varepsilon\eta_2)$, *and* $b^1(x), b^2(x)$ *denote the matrices formed by the first* $\bar{p}$ *and last* $p - \bar{p}$ *columns of* $b(x)$, *respectively.*

4. APPLICATIONS

In this section, we study two representative examples of a wide variety of chemical processes that exhibit time-scale multiplicity and are naturally modeled in the form of eq. (2). Our objectives are: (i) to illustrate the application of the proposed modeling methodology in deriving standard singularly perturbed representations of these processes, (ii) evaluate the performance of well-conditioned controllers synthesized on the basis of these representations, and (iii) illustrate the limitations of standard inversion-based controllers designed without taking into account the presence of time-scale multiplicity.

4.1. *A CSTR with heating jacket*

Consider a CSTR with heating jacket shown in Fig. 1. Reactant A is fed to the reactor at a flowrate

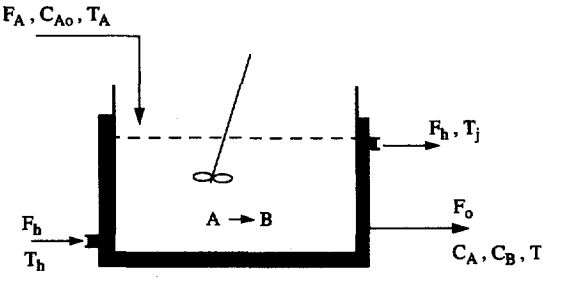

Fig. 1. A continuous-stirred tank reactor with heating jacket.

F_A, molar concentration C_{A0} and temperature T_A. The reactant A is converted into the product B through the irreversible endothermic reaction $A \rightarrow B$, and the product stream is withdrawn at a flowrate $F_0 = F_A$, i.e. the reactor holdup volume V is constant. The reaction rate r_A, is given by the following Arrhenius expression:

$$r_A = k_0 e^{(-E/RT)} C_A V$$

where k_0 and E are the reaction rate coefficient and activation energy, respectively, T is the reactor temperature, and C_A is the molar concentration of A in the reactor. Heat is provided to the reactor from the jacket, where a heating fluid is fed at a flowrate F_h and a temperature T_h. The modeling equations for the process include the mole balances for the two components in the reactor and the enthalpy balances in the reactor and the jacket. The resulting dynamic model is given by

$$\begin{aligned}
\dot{C}_A &= \frac{F_A}{V}(C_{A0} - C_A) - k_0 e^{(-E/RT)} C_A \\
\dot{C}_B &= -\frac{F_A}{V} C_B + k_0 e^{(-E/RT)} C_A \\
\dot{T} &= \frac{F_A}{V}(T_A - T) - k_0 e^{(-E/RT)} C_A \frac{\Delta H_r}{\rho c_p} \\
&\quad + \frac{UA}{\rho c_p}\left(\frac{T_j - T}{V}\right) \\
\dot{T}_j &= \frac{F_h}{V_h}(T_h - T_j) - \frac{UA}{\rho_h c_{ph}}\left(\frac{T_j - T}{V_h}\right).
\end{aligned} \tag{14}$$

It is assumed that the density and specific heat capacities of the two liquids are the same, i.e. $\rho_h = \rho$ and $c_{ph} = c_p$, and the liquid holdup in the jacket at a temperature T_j has a constant volume V_h. Furthermore, we consider the case when the heat transfer between the heating jacket and the reactor, $Q = UA(T_j - T)$, is fast compared to the reaction, i.e. $(UA/\rho c_p) = (1/\varepsilon)$. The values of the process parameters and variables at the nominal steady state are given in Table 1. It was verified that they correspond to a stable steady state.

For the process, it is desired to control the product concentration C_B and reactor temperature T using the reactant flowrate F_A and the heating fluid flowrate

Table 1. Nominal values of variables for reactor with heating jacket

Variable	Description	Nominal value
C_{A0}	Feed reactant concentration (mol/l)	2.5
C_A	Reactant concentration in reactor (mol/l)	1.205
C_B	Product concentration in reactor (mol/l)	1.295
c_p	Specific heat capacity (J/g K)	8.0
E	Activation energy (J/mol K)	60,000
F_A	Outlet flowrate from reactor (l/s)	2.0
F_h	Heating fluid flowrate (l/s)	0.1
k_0	Pre-exponential factor in reaction rate (s^{-1})	5×10^{10}
T_A	Feed reactant temperature (K)	305
T	Reactor temperature (K)	302.3
T_h	Heating fluid temperature (K)	330
T_j	Jacket temperature (K)	302.6
V	Reactor holdup volume (l)	1.0
V_h	Jacket volume (l)	0.2
ρ	Liquid density (g/l)	800
ΔH_r	Heat of reaction (J/mol)	20,000
ε	Small parameter ($\rho c_p/UA$) (s/l)	0.1

F_h as the manipulated inputs. Under the above conditions, the system of eq. (14) takes the form of eq. (2) with the states $x_1 = C_A, x_2 = C_B, x_3 = T, x_4 = T_j$, the manipulated inputs $u_1 = F_A$, $u_2 = F_h$, the controlled outputs $y_1 = x_2$, $y_2 = x_3$,

$$f(x) = \begin{bmatrix} -k_0 e^{(-E/Rx_3)}x_1 \\ k_0 e^{(-E/Rx_3)}x_1 \\ -k_0 e^{(-E/Rx_3)}x_1\left(\dfrac{\Delta H_r}{\rho c_p}\right) \\ 0 \end{bmatrix},$$

$$g(x) = \begin{bmatrix} \dfrac{(C_{A0} - x_1)}{V} & 0 \\ -\dfrac{x_2}{V} & 0 \\ \dfrac{(T_A - x_3)}{V} & 0 \\ 0 & \dfrac{(T_h - x_4)}{V_h} \end{bmatrix}, \quad b(x) = \begin{bmatrix} 0 \\ 0 \\ \dfrac{1}{V} \\ -\dfrac{1}{V_h} \end{bmatrix}$$

and $k(x) = x_4 - x_3$.

Let us first address the control of this process within a standard input/output linearization framework, ignoring its two-time-scale behavior. For the full model in eq. (14), the relative orders (see the appendix for the definition of relative order) of the two outputs y_1, y_2 with respect to the manipulated input vector u are $r_1 = 1, r_2 = 1$, respectively. However, both outputs are affected more directly by the same input u_1, and thus the characteristic matrix is singular (see the appendix for the definition of characteristic matrix). This implies the need for a dynamic feedback controller, which is designed by defining $v_1 = \dot{u}_1$ as a new manipulated input to obtain a system with an extended state vector $\bar{x} = [x^T \; u_1]^T$, new inputs $v_1 = \dot{u}_1, v_2 = u_2$, relative orders $r_1 = 2$, $r_2 = 2$, and a characteristic matrix that is nonsingular (the reader may refer to Isidori, 1995 for details). An input/output linearizing dynamic state feedback controller can be designed on the basis of the extended system to induce a well-characterized closed-loop response. Owing to the fact that the relative orders of both outputs in the extended system are two, the resulting controller involves terms multiplied by the large factors $(1/\varepsilon)$, $(1/\varepsilon^2)$ and thus it is severely ill-conditioned as illustrated through simulations later in this section.

We now address the control of the process accounting for its two-time-scale behavior within the proposed modeling framework. It is clear that in the limit $\varepsilon \to 0$, the heat transfer resistance becomes negligible and the reactor and jacket approach thermal equilibrium, i.e. $T_j \to T$. In this limiting case, the heat transfer rate Q is governed by the thermal equilibrium condition $T = T_j$ instead of the explicit heat transfer correlation. Thus, the algebraic variable is defined as $z = \lim_{\varepsilon \to 0}((T_j - T)/\varepsilon)$ to obtain a DAE representation of the slow dynamics of the form in eq. (4), for which $L_b k(x)$ is a scalar term that is nonzero. Furthermore, the one-dimensional distribution $B(x) = \text{span}\{b(x)\}$ is trivially involutive. Thus, the coordinate change of Theorem 1 takes the form

$$\begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \eta \end{bmatrix} = T(x) = \begin{bmatrix} x_1 \\ x_2 \\ Vx_3 + V_h x_4 \\ x_4 - x_3 \end{bmatrix}.$$

In the transformed coordinates, the two-time-scale system of eq. (14) has the following standard form:

$$\dot{\zeta}_1 = -r(\zeta, \eta) + \frac{(C_{A0} - \zeta_1)}{V}u_1$$

$$\dot{\zeta}_2 = r(\zeta, \eta) - \frac{\zeta_2}{V}u_1$$

$$\dot{\zeta}_3 = -r(\zeta, \eta)\left(\frac{V\Delta H_r}{\rho c_p}\right) + \left(T_A - \frac{\zeta_3 - V_h\eta}{V + V_h}\right)u_1 + \left(T_h - \frac{\zeta_3 + V\eta}{V + V_h}\right)u_2$$

$$\varepsilon\dot{\eta} = \varepsilon\left\{r(\zeta, \eta)\left(\frac{\Delta H_r}{\rho c_p}\right) - \frac{1}{V}\left(T_A - \frac{\zeta_3 - V_h\eta}{V + V_h}\right)u_1 + \frac{1}{V_h}\left(T_h - \frac{\zeta_3 + V\eta}{V + V_h}\right)u_2\right\} - \left(\frac{1}{V_h} + \frac{1}{V}\right)\eta$$

$$y_1 = \zeta_2$$

$$y_2 = \frac{\zeta_3 - V_h\eta}{V + V_h} \tag{15}$$

where $\zeta_1, \zeta_2, \zeta_3$ denote the slow variables, η is the fast variable and $r(\zeta, \eta) = k_0 e^{(-E(V+Vh)/R(\zeta_3 - V_h\eta))}\zeta_1$. Note that the controlled output y_2 explicitly depends on the fast variable η, i.e. the small deviation between the jacket and reactor temperatures. For the two-time-scale system of eq. (15), the one-dimensional fast subsystem is obtained by setting $\varepsilon = 0$ in the fast time scale τ

$$\frac{d\eta}{d\tau} = -\left(\frac{1}{V_h} + \frac{1}{V}\right)\eta$$

which is clearly exponentially stable at $\eta = 0$ since $V_h, V > 0$. Thus, the fast and stable subsystem can be ignored and a controller can be designed on the basis of the three-dimensional slow subsystem, obtained by setting $\varepsilon = 0$ in the slow time-scale t:

$$\dot{\zeta}_1 = -r(\zeta, 0) + \frac{(C_{A0} - \zeta_1)}{V}u_1$$

$$\dot{\zeta}_2 = r(\zeta, 0) - \frac{\zeta_2}{V}u_1$$

$$\dot{\zeta}_3 = -r(\zeta, 0)\left(\frac{V\Delta H_r}{\rho c_p}\right) + \left(T_A - \frac{\zeta_3}{V + V_h}\right)u_1 + \left(T_h - \frac{\zeta_3}{V + V_h}\right)u_2$$

$$y_{1s} = \zeta_2$$

$$y_{2s} = \frac{\zeta_3}{V + V_h}. \tag{16}$$

Note that in the slow subsystem, $\eta \equiv 0$, i.e. $T_j = T$ — a thermal equilibrium condition, analogous to the phase equilibrium conditions in multi-phase systems with a fast inter-phase mass transfer. Furthermore, in the slow subsystem, the controlled output $y_{1s} = y_1$, whereas $y_{2s} = (\zeta_3/(V + V_h))$ approximates the true reactor temperature T with the weighted average of the reactor and jacket temperatures, which is in accordance with the thermal equilibrium condition. It can be easily verified that in the slow subsystem of eq. (16), the relative orders of y_{1s} and y_{2s} with respect to the input vector u are $r_1 = 1$ and $r_2 = 1$, respectively, the corresponding characteristic matrix is nonsingular, and the one-dimensional zero dynamics of the slow subsystem is exponentially stable. Thus, an input/output linearizing controller with an external linear controller with integral action was designed, to induce the following decoupled first-order response in the slow subsystem:

$$y_{is} + \beta_{i1}^i \dot{y}_{is} = y_{isp}, \quad i = 1, 2 \tag{17}$$

where $\beta_{11}^1 = 10$ and $\beta_{21}^2 = 15$. The performance and robustness of this controller was compared with that of the controller synthesized on the basis of the full process model to induce the following decoupled second-order responses:

$$y_i + \beta_{i1}^i \dot{y}_i + \beta_{i2}^i \ddot{y}_i = y_{isp}, \quad i = 1, 2 \tag{18}$$

with the parameters tuned for critically damped responses with the same time constants as in the response of eq. (17), i.e. $\beta_{11}^1 = 20, \beta_{12}^1 = 100, \beta_{21}^2 = 30, \beta_{22}^2 = 225$.

The first run was used to study the performance of the two controllers in the nominal process, for a 15% increase in the setpoint for y_1. The corresponding profiles for the controlled outputs and the manipulated inputs are shown in Fig. 2. Clearly, the controller designed on the basis of the full model [eq. (14)] induces the decoupled second-order responses in the nominal process, as expected. The proposed controller based on the slow subsystem also yields excellent performance in this case.

The second run was performed for the same setpoint change, in the presence of a 5% error in the process parameters ΔH_r, ρ and c_p. The corresponding profiles are shown in Fig. 3. Clearly, the controller designed on the basis of the slow subsystem successfully rejects the effects of these small parametric errors without much performance degradation, and the calculated control action is also close to the nominal case, establishing the fact that the controller is not sensitive to small errors. On the other hand, the controller that ignored the time-scale multiplicity was very sensitive to these errors, since the effects of the small errors were magnified through the large factors $(1/\varepsilon), (1/\varepsilon^2)$ in the control law. As a result, the controller calculates a very large control action in the presence of these small modeling errors, leading to instability. These simulations clearly illustrate the problem of ill-conditioning in controllers designed through standard inversion-based approaches ignoring the time-scale-multiplicity of the process.

4.2. *A CSTR with multiple reactions in series*

The proposed modeling methodology will be now applied to the control of a CSTR where multiple fast and slow reactions take place. Consider a CSTR where reactant A is fed at a flow rate F_A, molar concentration C_{Ai} and temperature T_i, and the following reactions occur in series:

$$A \rightleftharpoons B \rightarrow C \rightarrow D$$

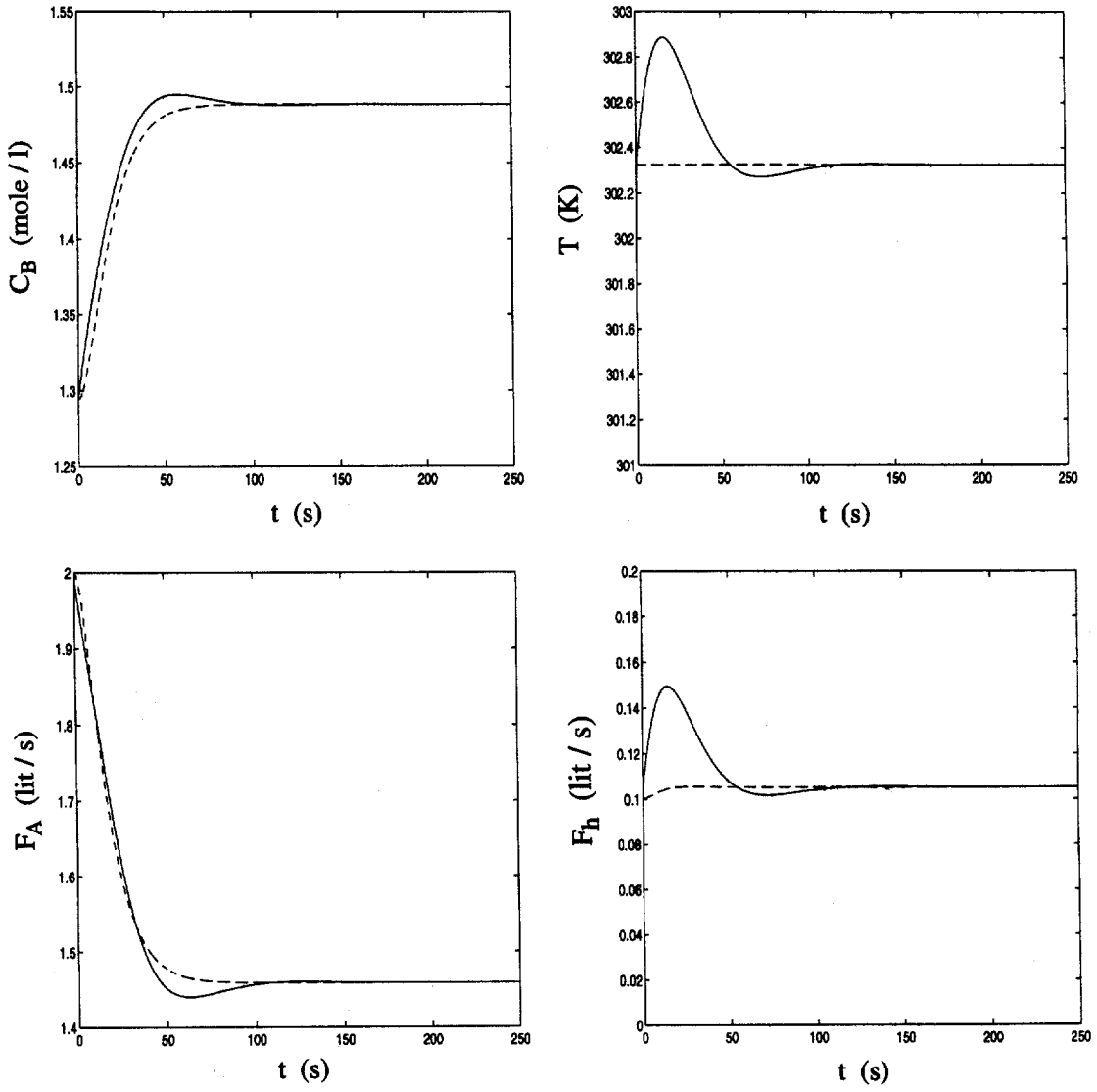

Fig. 2. Closed-loop responses with full- (dashed) and reduced-order (solid) model-based controllers for a 15% increase in y_{sp1}.

with B as the desired product. The reaction rate for the reversible reaction $A \rightleftharpoons B$ is given by $r_1 = k_1(C_A - (C_B/\kappa_1))$ where k_1 and κ_1 are the reaction rate and equilibrium constants at a temperature T, and C_A and C_B are the molar concentrations of A and B, respectively. The reaction rates for the irreversible reactions $B \rightarrow C$ and $C \rightarrow D$ are given by $r_2 = k_2 C_B$, and $r_3 = k_3 C_C$, respectively, and the three reaction rate constants are given by the Arrhenius relation

$$k_i = k_i^0 \exp\left(\frac{E_i}{R}\left(\frac{1}{T^0} - \frac{1}{T}\right)\right), \quad i = 1, 2, 3$$

where the superscript '0' refers to their values at the reference temperature T^0 taken to be the nominal reactor temperature. The dynamic model of the process has the following form:

$$\begin{aligned}
\dot{C}_A &= \frac{F_A}{V}(C_{Ai} - C_A) - k_1\left(C_A - \frac{C_B}{\kappa_1}\right) \\
\dot{C}_B &= -\frac{F_A}{V}C_B + k_1\left(C_A - \frac{C_B}{\kappa_1}\right) - k_2 C_B \\
\dot{C}_C &= -\frac{F_A}{V}C_C + k_2 C_B - k_3 C_C \\
\dot{C}_D &= -\frac{F_A}{V}C_D + k_3 C_C \\
\dot{T} &= \frac{F_A}{V}(T_i - T) - k_1\left(C_A - \frac{C_B}{\kappa_1}\right)\frac{\Delta H_{r1}}{\rho c_p} \\
&\quad - k_2 C_B \frac{\Delta H_{r2}}{\rho c_p} - k_3 C_C \frac{\Delta H_{r3}}{\rho c_p} - \frac{Q}{\rho V c_p}
\end{aligned} \tag{19}$$

where V, ρ, c_p are the holdup volume, density and specific heat capacity of the liquid, assumed constant.

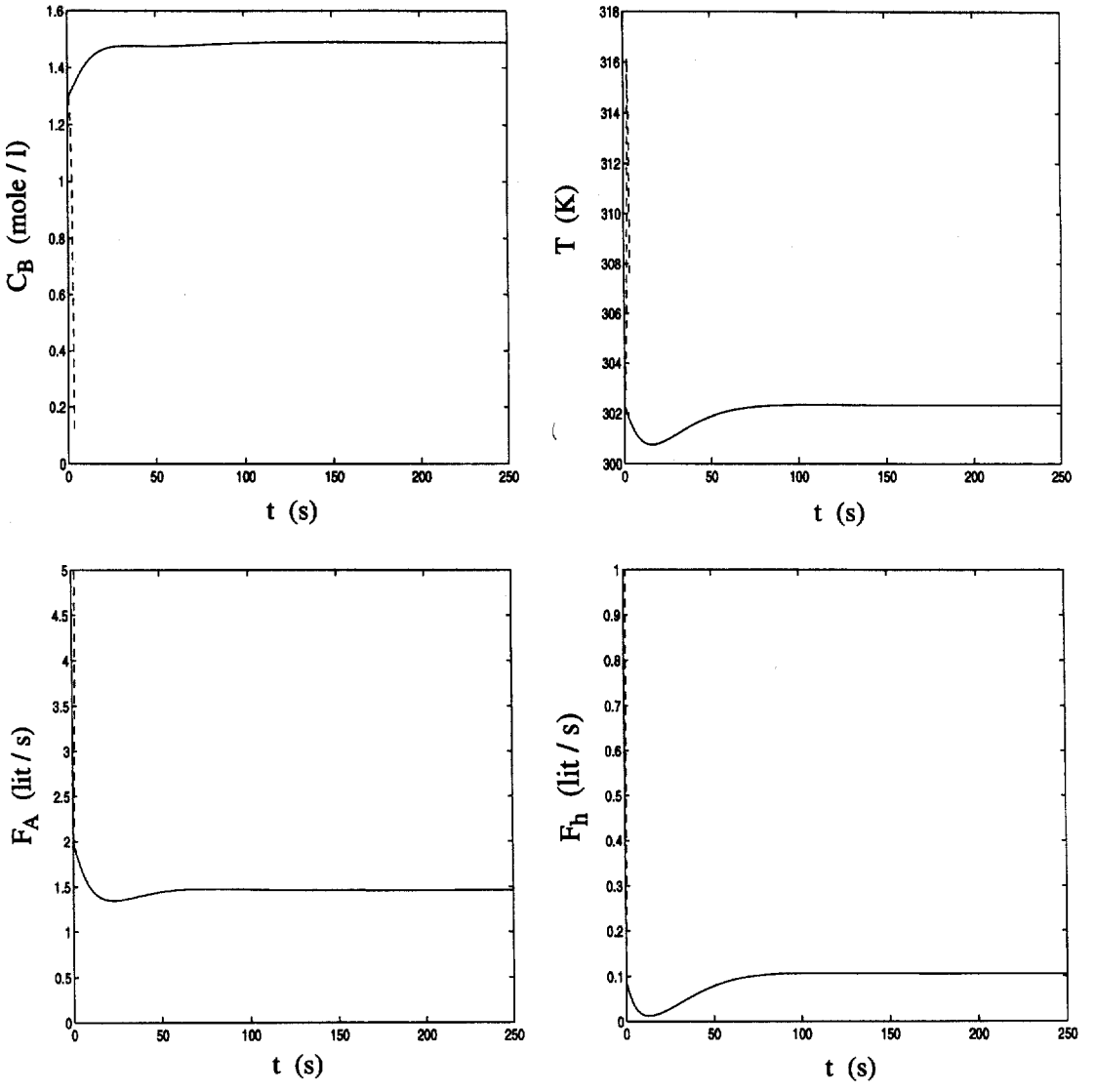

Fig 3. Closed-loop responses with full- (dashed) and reduced-order (solid) model-based controllers for a 15% increase in y_{sp1}, in the presence of 5% error in ΔH_r, ρ and c_p.

The heats of reaction at a temperature T are given by

$$\Delta H_{ri} = \Delta H_{ri}^0 + \Delta c_{pi}(T - T^0), \quad i = 1, 2, 3$$

where $\Delta c_{p1} = (c_{pB} - c_{pA})$, $\Delta c_{p2} = (c_{pC} - c_{pB})$, $\Delta c_{p3} = (c_{pD} - c_{pC})$, and $c_{pA}, c_{pB}, c_{pC}, c_{pD}$ are the molar heat capacities of the respective components. Furthermore, the reaction equilibrium constant κ_1 at the temperature T is governed by the following relation:

$$\ln\left(\frac{\kappa_1}{\kappa_1^0}\right) = \left(\frac{\Delta H_{r1}^0 - \Delta c_{p1} T^0}{R}\right)\left(\frac{1}{T^0} - \frac{1}{T}\right) + \left(\frac{\Delta c_{p1}}{R}\right) \ln\left(\frac{T}{T^0}\right).$$

For the process, it is desired to control the product concentration C_B and the reactor temperature T, using the reactant feed flow rate F_A and the heat duty Q as the manipulated inputs. The nominal values of the process parameters and variables are given in Table 2 and correspond to a stable steady state. As can be easily seen from Table 2, the first and third reactions are fast compared to the intermediate reaction, i.e. $k_1^0 \gg k_2^0$ and $k_3^0 \gg k_2^0$. Defining the small parameter $\varepsilon = (1/k_1^0)$ and an additional parameter $\kappa_2 = (k_3^0/k_1^0)$ where $\kappa_2 = O(1)$, the model in eq. (19) takes the form of the system in eq. (2) with the state variables $x_1 = C_A$, $x_2 = C_B$, $x_3 = C_C$, $x_4 = C_D$, $x_5 = T$, the manipulated inputs $u_1 = F_A$, $u_2 = Q$, the controlled outputs $y_1 = x_2$, $y_2 = x_5$, and

$$f(x) = \begin{bmatrix} 0 \\ -k_2 x_2 \\ k_2 x_2 \\ 0 \\ -\dfrac{k_2 x_2 \Delta H_{r2}}{\rho c_p} \end{bmatrix},$$

Table 2. Nominal values of variables for reactor with multiple reactions

C_{Ai}	10.0 mol/l	C_A	2.325 mol/l
C_B	5.756 mol/l	C_C	0.003 mol/l
C_D	1.916 mol/l	c_p	5.0 kJ/kg K
c_{pA}	120 J/mol K	c_{pB}	80 J/mol K
c_{pC}	70 J/mol K	c_{pD}	140 J/mol K
E_1	45 kJ/mol	E_2	35 kJ/mol
E_3	40 kJ/mol	F_A	3.0 l/min
k_1^0	100 min^{-1}	k_2^0	0.1 min^{-1}
k_3^0	200 min^{-1}	T	300 K
T_i	290 K	Q	58.42 kJ/min
V	10 l	κ_1^0	2.5
ρ	0.8 kg/l	ΔH_{r1}^0	−6.0 kJ/mol
ΔH_{r2}^0	−5.0 kJ/mol	ΔH_{r3}^0	−2.0 kJ/mol

$$k(x) = \begin{bmatrix} e^{E_1/R((1/T^0)-(1/x_5))}\left(x_1 - \dfrac{x_2}{\kappa_1}\right) \\ e^{E_3/R((1/T^0)-(1/x_5))}x_3 \end{bmatrix},$$

$$g(x) = \begin{bmatrix} \dfrac{C_{Ai}-x_1}{V} & 0 \\ -\dfrac{x_2}{V} & 0 \\ -\dfrac{x_3}{V} & 0 \\ -\dfrac{x_4}{V} & 0 \\ \dfrac{T_i - T}{V} & -\dfrac{1}{\rho V c_p} \end{bmatrix},$$

$$b(x) = \begin{bmatrix} -1 & 0 \\ 1 & 0 \\ 0 & -\kappa_2 \\ 0 & \kappa_2 \\ -\dfrac{\Delta H_{r1}}{\rho c_p} & -\dfrac{\kappa_2 \Delta H_{r3}}{\rho c_p} \end{bmatrix}.$$

Ignoring the two-time-scale behavior of the process, an input/output linearizing controller can be designed directly on the basis of the model in eq. (19). The relative orders of the two outputs y_1, y_2 with respect to the manipulated input vector u are $r_1 = 1$, $r_2 = 1$, and the characteristic matrix is nonsingular. However, the three-dimensional zero dynamics is also a two-time-scale system with two slow modes that are stable and a fast mode that is unstable, i.e., the process is slightly nonminimum phase (Isidori *et al.*, 1992). This is illustrated in Fig. 4, which shows an inverse response in y_1 in the boundary layer for a step increase in u_1, starting from the nominal steady state. Owing to this slightly nonminimum phase behavior, the above-mentioned controller leads to closed-loop instability, thereby highlighting the need for addressing the two-time-scale behavior in the design of a well-conditioned controller that yields a good performance with stability. Such a controller can be designed following the proposed singular perturbation modeling framework.

For the two-time-scale system, it is clear that as $\varepsilon \to 0$, $k(x) \to [0\ 0]^T$, i.e. $C_A \to (C_B/\kappa_1)$ and $C_C \to 0$. This is consistent with the physical intuition for processes with fast reactions, where reversible ones are essentially at equilibrium, and the irreversible ones correspond to pseudo-steady-state conditions of complete conversion of the reactants. With this observation, the two algebraic variables are defined as

$$z_1 = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} e^{(E_1/R)((1/T^0)-(1/x_5))}\left(x_1 - \frac{x_2}{\kappa_1}\right)$$

$$z_2 = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} e^{(E_3/R)((1/T^0)-(1/x_5))}x_3$$

to obtain a DAE representation of the slow dynamics, of the form in eq. (4), where the matrix $L_b k(x)$ is nonsingular. However, the two-dimensional distribution $B(x) = \text{span}\{b_1(x), b_2(x)\}$ is not involutive due to the fact that the heats of reaction ΔH_{r1} and ΔH_{r3} vary with the temperature T and the Lie bracket $[b_1(x), b_2(x)]$ (see the appendix for the definition) has the form $[0\ 0\ 0\ 0\ *]^T$ where '*' denotes a nonzero term. Thus, from Theorem 2, an ε-dependent coordinate change, singular at $\varepsilon = 0$, is required to obtain a standard form representation. Moreover, it can be verified that for $\bar{p} = 1$, condition (ii) of the proposition is not satisfied for *any* choice of the one-dimensional involutive distribution $\bar{B}(x) = \text{span}\{b_j(x)\}$ for $j = 1$ or $j = 2$, i.e. $L_{b_1}k_2(x) \not\equiv 0$, and $L_{b_2}k_1(x) \not\equiv 0$. Thus, both constraints $k_1(x) = 0$, $k_2(x) = 0$ have to be scaled by the factor $1/\varepsilon$ in the coordinate change

$$\begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \eta_1 \\ \eta_2 \end{bmatrix} = T(x, \varepsilon) = \begin{bmatrix} x_1 + x_2 \\ x_3 + x_4 \\ x_5 \\ \dfrac{1}{\varepsilon} e^{(E_1/R)((1/T^0)-(1/x_5))}\left(x_1 - \dfrac{x_2}{\kappa_1}\right) \\ \dfrac{1}{\varepsilon} e^{(E_3/R)((1/T^0)-(1/x_5))}x_3 \end{bmatrix}$$

to obtain a standard form representation of the form in eq. (11).

For the resulting system in the standard form, the two-dimensional fast subsystem is exponentially stable, uniformly in ζ, and the three-dimensional slow subsystem has the following representation

$$\dot{\zeta}_1 = -\frac{k_2\kappa_1}{1+\kappa_1}\zeta_1 + \frac{C_{Ai} - \zeta_1}{V}u_1$$

$$\dot{\zeta}_2 = \frac{k_2\kappa_1}{1+\kappa_1}\zeta_1 - \frac{\zeta_2}{V}u_1$$

$$\dot{\zeta}_3 = -\frac{k_2\kappa_1\zeta_1\Delta H_{r2}}{(1+\kappa_1)\rho c_p} + \left(\frac{T_i - \zeta_3}{V}\right)u_1 - \frac{u_2}{\rho V c_p} - \frac{\Delta H_{r1}}{\rho c_p}\eta_{1s} - \frac{\kappa_2 \Delta H_{r3}}{\rho c_p}\eta_{2s}$$

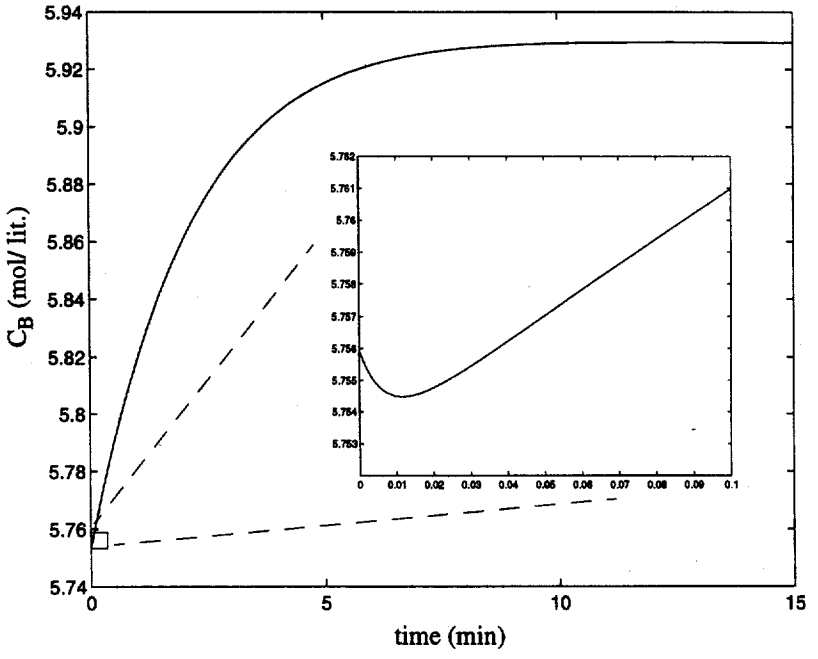

Fig. 4. Inverse response in C_B for step increase in F_A.

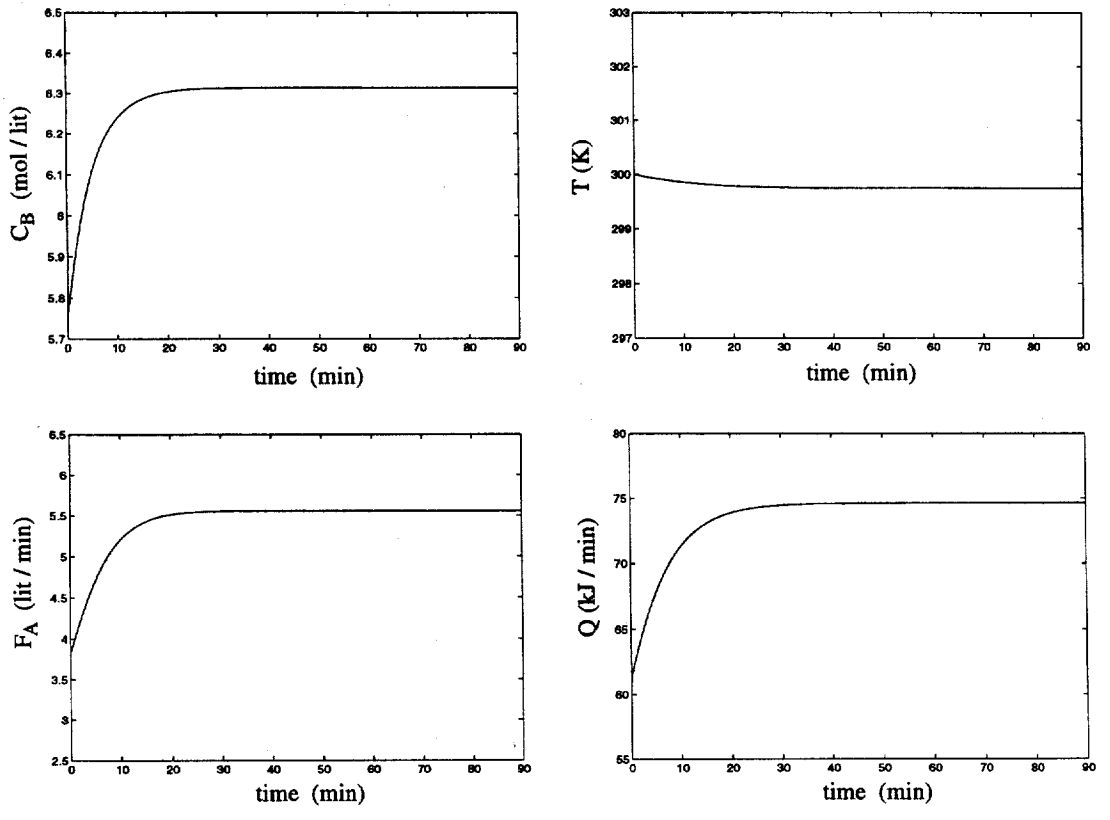

Fig. 5. Closed-loop profiles for a 10% increase in the set-point for C_B.

$$y_{1s} = \frac{\kappa_1}{1+\kappa_1}\zeta_1$$

$$y_{2s} = \zeta_3 \tag{20}$$

where $\eta_{1s} = \alpha_1(\zeta) + \alpha_2(\zeta)u_1 + \alpha_3(\zeta)u_2$ and $\eta_{2s} = (k_2\kappa_1\zeta_1/\kappa_2(\kappa_1+1))$ and the explicit form of $\alpha_1(\zeta)$, $\alpha_2(\zeta)$, $\alpha_3(\zeta)$ is omitted for brevity. For the above slow subsystem, the relative order of the two outputs

y_{1s}, y_{2s} are $r_1 = 1, r_2 = 1$, and the one-dimensional zero dynamics is locally exponentially stable. Thus, an input/output linearizing controller was designed on the basis of the slow subsystem in eq. (20), to induce the following decoupled first-order response in the closed-loop slow system:

$$y_{is} + \beta_i \dot{y}_{is} = y_{isp}, \quad i = 1, 2$$

with the parameters $\beta_1 = 5$ min and $\beta_2 = 8$ min. It was verified that the value of $\varepsilon = 0.01$ ensures that the output of the closed-loop system satisfies $y_i(t) = y_{is}(t) + O(\varepsilon)$, $t \geq 0$.

Figure 5 shows the closed-loop profiles of the controlled outputs and manipulated inputs, for a 10% increase in the setpoint for the first output y_{1sp}. The process at $t = 0$ was at the nominal steady state, which guarantees that $k_1(x) = O(\varepsilon)$ and $k_2(x) = O(\varepsilon)$. The profiles clearly show an excellent tracking performance with stability. The application study clearly demonstrates the effectiveness of the proposed singular perturbation modeling framework for the control of two-time-scale chemical processes that exhibit a slightly nonminimum phase behavior.

Remark 4: In the CSTR example, the slightly nonminimum phase behavior, in particular, the inverse response in the fast boundary layer (see Fig. 4), arises specifically due to the competition between the fast reaction $A \rightleftharpoons B$ and the slow reaction $B \rightarrow C$ in series, in the production of the intermediate component B which is the desired product. Such slightly nonminimum phase behavior arising due to a competition between the fast and slow phenomena may occur quite often in two-time-scale chemical processes, e.g. multi-phase reactors with a fast inter-phase mass transfer followed by a slow reaction in the reaction phase.

Remark 5: Note that for the CSTR example with multiple reactions, the controller synthesized on the basis of the slow subsystem does not require the values of the kinetic rate constants of the fast reactions, which may be difficult to obtain in practice. Only the kinetics of the slow reaction that essentially governs the process dynamics, and the thermodynamic equilibrium constant for the fast reversible reaction are required in the controller design. Similarly, in processes with fast mass transfer, heat transfer, etc., a knowledge of the mass/heat transfer rate coefficients is not required, rather the thermodynamic phase/thermal equilibrium relations are used in the controller design.

5. CONCLUSIONS

In this article, we proposed a framework for the singular perturbation modeling of two-time-scale chemical processes described by nonlinear ODEs that involve large parameters of the form $1/\varepsilon$. A result was initially derived that provides necessary and sufficient conditions for the existence and the explicit form of a coordinate change, which is independent of ε and transforms the two-time-scale process into a standard singularly perturbed form where the separation of fast and slow modes is explicit. Whenever these conditions are not satisfied, it was established that the state-space region in which the system exhibits a two-time-scale property depends on the value of ε and an ε-dependent coordinate change, singular at $\varepsilon = 0$, has to be employed to obtain a standard singularly perturbed form representation of the system, and the construction of such a transformation was addressed. The application of the proposed framework in deriving standard singularly perturbed representations and its significance in synthesizing well-conditioned controllers was demonstrated through chemical reactor applications.

Acknowledgements

Financial support for this work from NSF, Grant CTS-9320402, is gratefully acknowledged.

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APPENDIX

Consider the nonlinear system

$$\begin{aligned} \dot{x} &= f(x) + \sum_{j=1}^{m} g_j(x)\, u_j(t) \\ y_i &= h_i(x), \quad i = 1, \ldots, m \end{aligned} \tag{A1}$$

where $x \in X \subset \mathbb{R}^n$ is the vector of state variables, $f(x)$ and $g_j(x)$ denote analytic vector fields and $h_i(x)$ denote analytic scalar functions on X. We now recall the definitions of Lie derivative and Lie bracket, the definition of relative order (or relative degree) and characteristic (or decoupling) matrix, and the definition of involutivity for an m-dimensional distribution $G(x) = \text{span}\,\{g_1(x), \ldots, g_m(x)\}$. For further details, see, for example, Isidori (1995).

Definition 1: The Lie derivative $L_f h_i(x)$ of the scalar function $h_i(x)$ along the vector field $f(x)$ is defined as $L_f h_i(x) = (\partial h_i(x)/\partial x) f(x)$. Higher-order Lie derivatives are defined recursively as $L_f^k h_i(x) = L_f(L_f^{k-1} h_i(x))$.

Definition 2: The Lie bracket $[g_1(x), g_2(x)]$ of two vector fields $g_1(x)$ and $g_2(x)$ is a vector field defined as $[g_1(x), g_2(x)] = (\partial g_2(x)/\partial x) g_1(x) - (\partial g_1(x)/\partial x) g_2(x)$.

Definition 3: Referring to the system of eq. (A1), the relative order of the output y_i with respect to the input vector u is defined as the smallest integer r_i for which

$$[L_{g_1} L_f^{r_i - 1} h_i(x) \ \ldots \ L_{g_m} L_f^{r_i - 1} h_i(x)] \not\equiv [0 \ \ldots \ 0] \tag{A2}$$

or $r_i = \infty$ if such an integer does not exist.

Definition 4: The matrix

$$C(x) = \begin{bmatrix} L_{g_1} L_f^{r_1 - 1} h_1(x) & \cdots & L_{g_m} L_f^{r_1 - 1} h_1(x) \\ L_{g_1} L_f^{r_2 - 1} h_2(x) & \cdots & L_{g_m} L_f^{r_2 - 1} h_2(x) \\ \vdots & & \\ L_{g_1} L_f^{r_m - 1} h_m(x) & \cdots & L_{g_m} L_f^{r_m - 1} h_m(x) \end{bmatrix} \tag{A3}$$

is the characteristic matrix of the system of eq. (A1).

Definition 5: An m-dimensional distribution $G(x) = \text{span}\,\{g_1(x), \ldots, g_m(x)\}$ is involutive if the Lie bracket $[\tau_1, \tau_2]$ of any pair of vector fields belonging to $G(x)$ is a vector field which belongs to $G(x)$, i.e. for any $\tau_1 \in G(x), \tau_2 \in G(x)$, $[\tau_1, \tau_2] \in G(x)$.

Proof of Theorem 1: First, we will prove the necessity of the conditions (i) and (ii) for the existence of an ε-independent coordinate change that yields a representation of the system of eq. (2), in the standard singularly perturbed form. Thereafter, we prove the sufficiency through an explicit construction of such a coordinate change.

Necessity: Consider the two-time-scale system in eq. (2) for which there exists a nonlinear ε-independent coordinate change of the form

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x) = \begin{bmatrix} \alpha(x) \\ \beta(x) \end{bmatrix} \tag{A4}$$

where $\zeta \in \mathbb{R}^{n-\bar{p}}$ is the vector of slow variables, $\eta \in \mathbb{R}^{\bar{p}}$ is the vector of fast variables, and $\alpha(x), \beta(x)$ are smooth vector fields of dimensions $(n - \bar{p})$ and $\bar{p}$, respectively, such that in these transformed coordinates, the system has the following representation in the standard form:

$$\begin{aligned} \dot{\zeta} &= F^1(\zeta, \eta, u, \varepsilon) \\ \varepsilon\dot{\eta} &= F^2(\zeta, \eta, u, \varepsilon) \end{aligned} \tag{A5}$$

where

$$\begin{aligned} F^1(\zeta, \eta, u, \varepsilon) &= [L_f \alpha(x) + \frac{1}{\varepsilon} L_b \alpha(x)\, k(x) \\ &\quad + L_g \alpha(x) u]_{x = T^{-1}(\zeta, \eta)} \\ F^2(\zeta, \eta, u, \varepsilon) &= [\varepsilon L_f \beta(x) + L_b \beta(x)\, k(x) \\ &\quad + \varepsilon L_g \beta(x)\, u]_{x = T^{-1}(\zeta, \eta)}. \end{aligned} \tag{A6}$$

Note that $\bar{p}$ is an arbitrary integer less than n. It will be shown that, in fact, $\bar{p} = p$, i.e. the two-time-scale system in eq. (A5) has exactly p fast states and $n - p$ slow states.

For the system in eq. (A5), the $\bar{p} \times \bar{p}$ Jacobian $(\partial F^2(\zeta, \eta, u, 0)/\partial \eta)$ is nonsingular, where

$$\begin{aligned} F^2(\zeta, \eta, u, 0) &= L_b \beta(x) k(x)|_{x = T^{-1}(\zeta, \eta)} \\ &= \begin{bmatrix} L_{b_1} \beta_1(x) & \cdots & L_{b_{\bar{p}}} \beta_1(x) \\ \vdots & & \vdots \\ L_{b_1} \beta_{\bar{p}}(x) & \cdots & L_{b_{\bar{p}}} \beta_{n-\bar{p}}(x) \end{bmatrix} k(x)\,|_{x = T^{-1}(\zeta, \eta)}. \end{aligned}$$

From our previous analysis of the slow dynamics in the slow time-scale t, we know that $\lim_{\varepsilon \to 0} k(x) = 0$, i.e. $\hat{k}(\zeta, \eta) = k(x)_{x = T^{-1}(\zeta, \eta)} = 0$. Thus, the nonsingularity of the $\bar{p} \times \bar{p}$ Jacobian

$$\frac{\partial F^2(\zeta, \eta, u, 0)}{\partial \eta} = L_b \beta(x)|_{x = T^{-1}(\zeta, \eta)} \times \left(\frac{\partial \hat{k}(\zeta, \eta)}{\partial \eta} \right)$$

implies that the $\bar{p} \times p$, $p \times \bar{p}$ matrices $L_b \beta(x)$ and $(\partial \hat{k}(\zeta, \eta)/\partial \eta)$ have full ranks $\bar{p}$ and thus, $\bar{p} \leqslant p$. Furthermore, the two-time-scale system of eq. (A5) has the following representation in the fast time-scale τ

$$\begin{aligned} \zeta' &= \varepsilon F^1(\zeta, \eta, u, \varepsilon) \\ \eta' &= F^2(\zeta, \eta, u, \varepsilon) \end{aligned} \tag{A7}$$

where in the limit $\varepsilon \to 0$, the slow variables ζ are constant. This, together with the fact that $k(x)$ in the fast time-scale τ, is an arbitrary nozero vector field of dimension p, leads to the conclusion that

$$L_b \alpha(x) = \begin{bmatrix} L_{b_1} \alpha_1(x) & \cdots & L_{b_p} \alpha_1(x) \\ \vdots & & \vdots \\ L_{b_1} \alpha_{n-\bar{p}}(x) & \cdots & L_{b_p} \alpha_{n-\bar{p}} \ (x) \end{bmatrix} \equiv 0.$$

Equivalently, the $(n - \bar{p})$ gradient covector fields $(d\alpha_i(x)/dx)$, $i = 1, \ldots, (n - \bar{p})$ are orthogonal to the p-dimensional distribution $B(x) = \text{span}\,\{b_1(x), \ldots, b_p(x)\}$ and thus, $\bar{p} \geqslant p$. Clearly, in view of the previous inequality $\bar{p} \leqslant p$, it

directly follows that $\bar{p} = p$ and the distribution $B(x)$ is involutive, from Frobenius Theorem (Isidori, 1995). This proves the necessity of condition (ii). Furthermore, the $p \times p$ matrices

$$L_b\beta(x)|_{x=T^{-1}(\zeta,\eta)}, \quad \left(\frac{\partial \hat{k}(\zeta,\eta)}{\partial \eta}\right)$$

are nonsingular. With the above observations, a proof for condition (i) can be obtained by evaluating the $p \times p$ matrix $L_b k(x) = (\partial k(x)/\partial x)\, b(x)$ in the transformed coordinates (ζ, η)

$$\begin{aligned} L_b k(x)|_{x=T^{-1}(\zeta,\eta)} &= \left(\frac{\partial \hat{k}(\zeta,\eta)}{\partial \eta}\right)\left(\frac{\partial \beta(x)}{\partial x}\right) b(x) \\ &+ \left(\frac{\partial \hat{k}(\zeta,\eta)}{\partial \zeta}\right)\left(\frac{\partial \alpha(x)}{\partial x}\right) b(x)\Big|_{x=T^{-1}(\zeta,\eta)} \\ &= \left(\frac{\partial \hat{k}(\zeta,\eta)}{\partial \eta}\right) L_b\beta(x) + \left(\frac{\partial \hat{k}(\zeta,\eta)}{\partial \zeta}\right) L_b\alpha(x)\Big|_{x=T^{-1}(\zeta,\eta)} \end{aligned}$$

Clearly, from the fact that $L_b\alpha(x)|_{x=T^{-1}(\zeta,\eta)} \equiv 0$ and that the matrices $(\partial \hat{k}(\zeta,\eta)/\partial\eta)$, $L_b\beta(x)|_{x=T^{-1}(\zeta,\eta)}$ are nonsingular, it is evident that $L_b k(x)$ is also nonsingular, proving the necessity of condition (i).

Sufficiency: The sufficiency of conditions (i) and (ii) can be established through the construction of a nonlinear ε-independent coordinate change that yields the standard form representation in eq. (7). More specifically, from the Frobenius Theorem, the involutivity of the distribution $B(x)$ in condition (ii) implies the existence of exactly $(n-p)$ scalar functions $\phi_i(x)$, $i = 1, \ldots, (n-p)$ such that the gradient covector fields $(d\phi_i(x)/dx)$ are linearly independent and satisfy $(d\phi_i(x)/dx)\, b_j(x) \equiv 0$, $\forall j$. Moreover, the nonsingularity of $L_b k(x)$ in the condition (i) implies that

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x) = \begin{bmatrix} \phi(x) \\ k(x) \end{bmatrix}$$

is a valid local diffeomorphism, where $\phi(x) = [\phi_1(x \cdots \phi_{n-p}(x)]^T$. In these coordinates, the system of eq. (2) has the representation in eq. (7), which is in the standard form since the matrix $Q(\zeta, \eta, 0) = L_b k(x)_{x=T^{-1}(\zeta,\eta)}$ is nonsingular. This completes the proof of the sufficiency. □

Proof of Theorem 2: Under condition (i) of theorem 1, the system of eq. (2) has $n-p$ slow and p fast modes. Statement (i) is proved by contradiction. Assume that the system of eq. (2) exhibits a two-time-scale property in a region $\mathcal{M} \subset \mathcal{X}$ where $k_i(x) = O(1)$, $\forall i$, and $\dim \mathcal{M} = n$, independently of ε. This implies that there exists an ε-dependent coordinate change of the form

$$\begin{bmatrix} \zeta \\ \eta \end{bmatrix} = T(x, \varepsilon) = \begin{bmatrix} \phi(x, \varepsilon) \\ \psi(x, \varepsilon) \end{bmatrix} \tag{A8}$$

which is *not* singular at $\varepsilon = 0$, i.e. $T(x, 0)$ is a valid coordinate change, and yields a standard singularly perturbed form. Under the transformation of eq. (A8), the system of eq. (2) takes the form

$$\begin{aligned} \dot{\zeta} &= L_f\phi(x, \varepsilon) + L_g\phi(x, \varepsilon)u + \frac{1}{\varepsilon} L_b\phi(x, \varepsilon)\, k(x) \\ \varepsilon\dot{\eta} &= \varepsilon L_f\psi(x, \varepsilon) + \varepsilon L_g\psi(x, \varepsilon)u + L_b\psi(x, \varepsilon)\, k(x) \end{aligned} \tag{A9}$$

where $x = T^{-1}(\zeta, \eta, \varepsilon)$, and ζ and η are the slow and fast state vectors, respectively. The fact that ζ_j, $j = 1, \ldots, n-p$ are the slow variables, implies that in the fast time-scale $\tau = t/\varepsilon$, $(d\zeta_j/d\tau) = O(\varepsilon)$, and thus $L_b\phi_j(x, \varepsilon)k(x) = O(\varepsilon)$. However, since $B(x)$ is not involutive, at least one of the elements of the $(n-p) \times p$ matrix $L_b\phi(x, \varepsilon)$ is of $O(1)$, which directly implies that $k_i(x) = O(\varepsilon)$ for at least one $i \in [1, p]$, thus yielding a contradiction.

Regarding statement (ii) of the theorem, we have that the system in eq. (A9) is clearly not in the standard form since $\dot{\zeta}$ depends explicitly on the term $1/\varepsilon$, thereby establishing the necessity of a coordinate change that is singular at $\varepsilon = 0$. □