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On the nonlinear dynamic state reconstruction problem for chemical/biochemical reaction systems in the presence of model uncertainty

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A new approach to the unmeasurable state reconstruction problem for nonlinear chemical reaction systems in the presence of model uncertainty is proposed. In particular, a new robust nonlinear state estimation method is developed that explicitly uses all the available useful information associated with: (i) a dynamic model inevitably characterized by uncertainty, and (ii) a set of sensor measurements in order to accurately reconstruct other key quantities/variables that cannot be measured on-line due to physical and/or technical limitations. The problem of interest is conveniently formulated and addressed within the context of singular partial differential equations (PDE) theory, leading to a nonlinear state estimator that possesses a state-dependent gain computed through the solution of a system of first-order singular PDEs. A set of necessary and sufficient conditions is presented that ensure the existence and uniqueness of a locally analytic solution to the aforementioned system of singular PDEs, and a series solution method that can be easily implemented via a MAPLE code is developed. Under these conditions, the convergence of the estimation error or the mismatch between the actual unmeasurable states and their estimates is analyzed and characterized in the presence of model uncertainty. Finally, the performance of the proposed nonlinear etimator and its convergence properties are evaluated in an illustrative biochemical reaction system that exhibits nonlinear behavior coupled with parametric uncertainty, and the estimation objective is to accurately reconstruct the unmeasurable substrate concentration using the available cell mass concentration measurements and the model of the system under consideration.

KEY WORDS: chemical reaction systems, nonlinear dynamical systems, state estimation, model uncertainty, singular PDEs

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1. Introduction

Broad classes of chemical reaction systems exhibit nonlinear dynamic behavior and are typically modeled by systems of nonlinear differential equations [1–3]. These dynamic models aim at capturing the actual behavior of the system of interest as faithfullly as possible, and are now extensively used (simulated) in order to generate reliable predictions, as well as monitor the system's dynamic state for product quality (yield, selectivity, conversion, etc.) and/or process safety purposes (reactions with runaway potential, heat generated by exothermic reactions, ignition conditions, etc.) [2–11]. Furthermore, in order to meet the above objectives and characterize the chemical reaction system's behavior, the explicit use of such a dynamic model (in various degrees of complexity and descriptive accuracy) is often complemented by sensor measurements related to measurable physical and chemical quantities [4–6]. However, it is a rare occasion in practice for all variables to be available for direct on-line measurement due to physical and/or technical limitations pertaining to the current state of sensor technology [12,13]. In most cases there is a substantial need for an accurate estimation and dynamic reconstruction of key unmeasurable physical and chemical variables, especially when they are used for system performance monitoring purposes and in the design of advanced process control systems in the chemical industries [4,5,12,13]. For this particular task, a state estimator/observer or "software sensor" is usually employed and appropriately designed in order to accurately reconstruct the aforementioned unmeasurable variables. The state estimator/observer is a dynamic system itself which is driven by the available on-line sensor measurements, and capitalizes on the available information provided by the chemical system/process model [13–15]. The observer's dynamic equations are then simulated on-line with the aid of a computer code, and offer accurate estimates of the unmeasurable quantities (hence the name "software or soft sensors"). In the world of linear systems, both the well-known Kalman filter [16] and its deterministic analogue realized by Luenberger's observer [14,17], offer a full comprehensive solution to the problem. In the case of nonlinear systems, the traditional practical approach in designing state observers relies on a local linearization around the reference equilibrium point, and the subsequent employment of linear observer design methods [13,16]. However, this approach exhibits only local validity because it overlooks the dominant process nonlinearities, and as reported in [13], might lead to poor performance of the observer. Consequently, in order to overcome the above type of performance limitations, nonlinear observers need to be designed that can directly cope with the system nonlinearities [15]. It should be pointed out however, that the nonlinear observer design problem poses considerable challenges and has received appreciable attention in the pertinent body of literature. One could mention the extended Kalman filter and extended Luenberger observers, whose design is based on a local linearization of the system around a reference trajectory and the reconstructed state,

respectively [4,16]. Undoubtedly, the first systematic approaches for the development of a design method for nonlinear observers were reported in [18–20], where nonlinear coordinate transformations were proposed in order to linearize the original system followed by linear methods to complete the state observer design procedure. However, this linearization approach is based upon a set of rather restrictive conditions, that are only met in a very limited class of systems [15]. Other important contributions to the nonlinear observer design problem can be found in [21–31], where a different type of methodological approach is followed for classes of nonlinear systems exhibiting special structural characteristics. It should be pointed out, that dynamic models cannot fully capture and accurately describe the actual system's behavior in practice, due to the inevitable modeling errors and/or model uncertainty pertaining for example to unknown or poorly known kinetic parameter values [4,5,32]. It is therefore quite important to investigate the possibility of designing observers that are capable of providing robust and accurate estimates of the unmeasurabe quantities in the presence of model uncertainty and/or modeling errors [5,32]. In this direction, the present research work aims at the development of a new approach to the unmeasurable physical and/or chemical variable reconstruction problem for nonlinear chemical reaction systems in the presence of model uncertainty by following a technically different path of analysis. In particular, the problem under consideration is conveniently addressed within the context of singular partial differential equations (PDE) theory, leading to a nonlinear state observer that has a state-dependent gain computed through the solution of a system of first-order singular PDEs. A set of necessary and sufficient conditions is presented that ensures the existence and uniqueness of a locally analytic solution to the aforementioned system of singular PDEs, and a series solution method is developed that can be easily implemented via a MAPLE code. Under these conditions, the convergence of the estimation error (or the mismatch between the actual unmeasurable variables and their estimates) to zero is analyzed and characterized in the presence of model uncertainty.

The present paper is organized as follows: In section 2, the necessary mathematical prerequisites are briefly presented, as well as the formulation of the problem under consideration. The paper's main results are reported in section 3, where the requisite analysis on the behavior of the estimation error and the convergence properties of the proposed state observer in the presence of model uncertainty is also conducted. In section 4, the performance of the proposed nonlinear observer is evaluated in an illustrative biochemical reaction system that exhibits nonlinear behavior along with parametric uncertainty, and the estimation objective is to accurately reconstruct the unmeasurable substrate concentration profile using the available cell mass concentration measurements and the system's model. Finally, some concluding remarks are provided in Section 5.

2. Mathematical preliminaries—problem formulation

In the present study spatially homogeneous chemical reaction systems are considered, which are realized by the following M chemical reactions involving S species:

$$\sum_{j=1}^{S} \nu_{ij} A_j \rightleftharpoons 0, \tag{1}$$

where $i = 1, \ldots, M$ and ν_{ij} denotes the stoichiometric coefficient of the j-th species A_j in the i reaction. It is assumed that the above chemical reactions take place in a standard continuous stirred-tank reactor (CSTR) and constitute a constant volume reacting mixture [3,6]. If r_i and ΔH_i denote the reaction rate and the heat of chemical reaction i, respectively, the dynamics of the system under consideration can be derived from standard mass and energy balances and mathematically realized by a system of nonlinear ordinary differential equations (ODEs) describing the evolution of the various species concentrations, as well as the reacting mixture temperature inside the chemical reactor [6,33]:

$$\begin{aligned} \frac{\mathrm{d}C_j}{\mathrm{d}t} &= \sum_{i=1}^{M} \nu_{ij} r_i + \frac{F}{\rho V}(C_j^{\mathrm{in}} - C_j), \\ \frac{\mathrm{d}T}{\mathrm{d}t} &= -\frac{1}{\rho C_p} \sum_{i=1}^{M} \Delta H_i r_i + \frac{F C_p^{\mathrm{in}}}{\rho V C_p}(T^{\mathrm{in}} - T) + \frac{UA}{\rho V C_p}(T^{\mathrm{h}} - T). \end{aligned} \tag{2}$$

In the above mathematical representation C_j denotes the concentration of species j ($j = 1, \ldots, S$), T the reactor temperature, V, C_p, ρ, the volume, heat capacity and density of the reacting mixture respectively, F denotes the mass flowrate, U and A denote the heat transfer coefficient and area, respectively, T^{h} denotes the temperature of the heat transfer medium, and finally the superscript "in" denotes quantities associated with the inlet stream. System (2) can be mathematically represented in a more compact form if vectorial/matrix notation is used. Indeed, let us collectively define the vector of variables:

$$x = \begin{bmatrix} C_1 \\ \cdot \\ \cdot \\ \cdot \\ C_S \\ T \end{bmatrix},$$

that is often called the state vector (equivalently the vector of state variables), since it uniquely determines and characterizes the dynamic state of the chemical reaction system of interest as its evolution is deterministically governed by the system of ODEs (2) [34–36]. Furthermore, one may define:

(i) the M-dimensional reaction rate vector:

$$r(x) = \begin{bmatrix} r_1 \\ \cdot \\ \cdot \\ \cdot \\ r_M \end{bmatrix},$$

where each reaction rate r_i is typically expressed as follows: $r_i = k_i(T)\tilde{r}_i(C)$, with $k_i(T)$ being the temperature-dependent kinetic rate constant [6,33].

(ii) the $(S+1) \times M$-dimensional generalized stoichiometric matrix [33]:

$$N(x) = \begin{bmatrix} \nu_{11} & \cdots & \nu_{M1} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \nu_{1S} & \cdots & \nu_{MS} \\ \frac{-\Delta H_1}{\rho C_p} & \cdots & \frac{-\Delta H_M}{\rho C_p} \end{bmatrix}$$

(iii) the vector function: $J(x)$, $J : R^{S+1} \longrightarrow R^{S+1}$ that captures all remaining terms in (2) associated with mass flow and heat transfer [6,33]:

$$J(x) = \begin{bmatrix} \frac{F}{\rho V}(C_1^{\text{in}} - C_1) \\ \cdot \\ \cdot \\ \cdot \\ \frac{F}{\rho V}(C_S^{\text{in}} - C_S) \\ \frac{FC_p^{\text{in}}}{\rho V C_p}(T^{\text{in}} - T) + \frac{UA}{\rho V C_p}(T^{\text{h}} - T) \end{bmatrix}.$$

Using the above notation, system (2) attains the following form:

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = N(x(t))r(x(t)) + J(x(t)) \equiv F(x(t)), \tag{3}$$

where $F(x)$, $F : R^{S+1} \longrightarrow R^{S+1}$ is used to denote the vector function appearing on the right hand-side of the above system of ODEs. In the context of the present study, it is assumed that $x \in X \subset R^{S+1}$, where X is a compact subset of the state space (it is therefore implicitly assumed that only stable dynamical systems (3) are considered with bounded state space trajectories $x(t)$ contained in X, otherwise, it is presupposed that a controller has been synthesized to render the controlled chemical system/process stable), and that $F(x)$ is a real analytic vector function on X. For the sake of simplicity and without loss of generality, the origin $x^0 = 0$ is assumed to be an equilibrium point of (3). Indeed, in the case of a non-zero equilibrium point: $x^0 \neq 0$, a simple linear transformation (axis shift) : $\tilde{x} = x - x^0$, with $\tilde{F}(\tilde{x}) \equiv F(\tilde{x} + x^0)$, maps the above non-zero equilibrium

point to the origin in the new coordinate system, where the system dynamics is represented in a formalistically similar manner as follows:

$$\frac{\mathrm{d}\tilde{x}(t)}{\mathrm{d}t} = \tilde{F}(\tilde{x}(t)). \tag{4}$$

In light of the above remark, the original notation will be retained for simplicity.

As it is often the case in practice, the above dynamic model can not adequately capture and faithfully describe the behavior of the actual system over all possible regimes of dynamic behavior due to model uncertainty that is inevitably introduced in modeling efforts. For example, one may envision cases where kinetic parameters in chemical reaction systems are unknown or poorly known, and thus responsible for an element of uncertainty in the dynamic description of the system under consideration [3–6, 13]. Mathematically, this uncertainty is very often represented in the following fashion:

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = F(x(t)) = f(x(t)) + \varepsilon g(x(t)), \tag{5}$$

where the $F(x)$ vector function is now partitioned into two terms: $F(x) = f(x) + \epsilon g(x)$. The first term: $f(x)$, with $f(0) = 0$, is the "known" part of the dynamic model (or equivalently its nominal part), and the second one: $\epsilon g(x)$ represents the model uncertainty or modeling error. Please notice, that $\epsilon > 0$ is typically a small number (perturbation parameter) and even though we do not know $g(x)$ exactly, we do have some knowledge about it, for example some type of bound. Indeed, it is often assumed that the perturbation term $g(x)$ is bounded on X and satisfies the following condition:

$$||g(x)|| \leqslant M, \tag{6}$$

where $M > 0$ and $x \in X$.

Let us now assume that $m < (S + 1)$ quantities: $y \in R^m$, $y = [y_1, \ldots, y_m]$ are available for direct on-line measurement and mathematically represented as functions of the state variables: $y = h(x)$, where $h : R^{S+1} \longrightarrow R^m$ is a real analytic vector function. Even though this is a rather generic representation, very often y is a subset of the state variables that can be measured with the aid of current sensor technology listed as: $y = [x_1, \ldots, x_m]$, whereas the rest $(S + 1 - m)$ variables: $[x_{m+1}, \ldots, x_{S+1}]$ are unmeasurable and need to be accurately reconstructed for product quality, process safety and/or other performance monitoring purposes. For example, it is easier to obtain fast and reliable temperature measurements than concentration measurements , or cell mass concentration measurements than substrate concentration and enzymatic concentration measurements in biochemical reaction systems [3–6, 12, 13].

Suppose now that for the "known" nominal dynamic model accompanied by the sensor measurement signals:

$$\begin{aligned} \frac{\mathrm{d}x(t)}{\mathrm{d}t} &= f(x(t)), \\ y(t) &= h(x(t)), \end{aligned} \tag{7}$$

one can design a state estimator or observer:

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = w(\hat{x}(t), y(t)), \tag{8}$$

which is a dynamical system itself, driven by the available sensor measurements $y(t)$ and capable of providing accurate estimates $\hat{x}(t)$ of the state vector $x(t)$, in the sense that the estimation error: $e(t) = x(t) - \hat{x}(t)$ (or the mismatch between the state x and its estimate $\hat{x}$) converges to zero asymptotically: $||e(t)|| = ||x(t) - \hat{x}(t)|| \longrightarrow 0$, as $t \longrightarrow \infty$. It is therefore understood, that the convergence properties of the above state estimator or state observer are dictated by the choice of the vector function $w(\hat{x}, y)$ on the right-hand-side of the observer's dynamic equations (8). This particular choice should enforce a decaying over time dynamic profile for the estimation error $e(t)$, and preferrably assign stable, smooth and fast dynamic modes to the estimation error dynamics. Equivalently stated, the choice of $w(\hat{x}, y)$ should induce the desirable speed/rate of convergence of the state estimate $\hat{x}$ to the actual state x. In light of the above remarks, an important question naturally arises: Would the aforementioned observer still offer a reliable state vector estimate $\hat{x}$ that converges to the actual state x in the presence of model uncertainty $g(x)$, and therefore exhibit convergence properties that are robust to modeling errors and uncertainty? Mathematically stated, under what conditions the estimation error dynamics is structurally stable in the presence of the perturbation term $\varepsilon g(x)$, or equivalently, the stability of the error dynamics is robust in the presence of model uncertainty/error? The study of this problem is the subject of section 3.

3. Main results

At this point it would be methodologically appropriate to first consider and study the state estimator design problem for the nominal unperturbed system (7) as presented in [37]. This is necessary, since it will form the basis for the ensuing framework of analysis where the robustness properties of the proposed state estimation method will be examined in the presence of model uncertainty for

nonlinear chemical reaction systems. At this point, let the Jacobian matrix F of the $f(x)$ vector function evaluated at $x = 0$ be denoted as: $F = (\partial f/\partial x)(0)$, and by H the $m \times (S+1)$ matrix: $H = (\partial h/\partial x)(0)$. For the nominal unperturbed system (7), we consider a nonlinear state observer of the following form:

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = w(\hat{x}(t), y(t)) = f(\hat{x}(t)) + L(\hat{x}(t))(y(t) - h(\hat{x})(t)), \tag{9}$$

where $\hat{x} \in R^{S+1}$ is the state estimate. The above observer is comprised of two terms: the first one: $f(\hat{x})$ is a replica of the nominal system dynamics (7), and the second term: $L(\hat{x}(t))(y(t) - h(\hat{x})(t))$ (which drives the observer dynamics (9)) is a "feedback term" that accounts for the mismatch between the actual sensor measurement $y(t)$ and the estimate of the measured quantities $h(\hat{x}(t))$ multiplied by a state-dependent "gain" $L(\hat{x})$. Let us now compute the gain map $L(x)$ as follows:

$$L(x) = \left[\frac{\partial T}{\partial x}(x)\right]^{-1} B, \tag{10}$$

where $T(x)$, $T : R^{S+1} \longrightarrow R^{S+1}$ is the solution to the following associated system of first-order partial differential equations (PDEs):

$$\begin{aligned} &\frac{\partial T}{\partial x} f(x) = AT(x) + Bh(x), \\ &T(0) = 0 \end{aligned} \tag{11}$$

with A, B being constant matrices of appropriate dimensions. Please notice, that under the above choice of the nonlinear gain $L(x)$, the state observer (9) induces the following linear error dynamics in the transformed coordinates $z = T(x)$:

$$\begin{aligned} \frac{\mathrm{d}e_z}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}(z - \hat{z}) = \frac{\mathrm{d}}{\mathrm{d}t}(T(x) - T(\hat{x})) = \frac{\partial T}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\partial T}{\partial \hat{x}}\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} \\ &= \frac{\partial T}{\partial x} f(x) - \frac{\partial T}{\partial \hat{x}}\{f(\hat{x}) + L(\hat{x})(y - h(\hat{x}))\} \\ &= AT(x) + Bh(x) - AT(\hat{x}) - Bh(\hat{x}) - Bh(x) + Bh(\hat{x}) \\ &= A(T(x) - T(\hat{x})) = A(z - \hat{z}) = Ae_z. \end{aligned} \tag{12}$$

Therefore, if in the above linear error dynamics the fundamental matrix A is chosen to have stable eigenvalues (Hurwitz matrix), these eigenvalues will directly regulate the exponential rate of decay of the estimation error: $e_z(t) = z(t) - \hat{z}(t) = T(x(t))) - T(\hat{x}(t)$ to zero (eigenmodes of the estimation error dynamics (12)). Notice, that invertibility of the matrix $\partial T/\partial x$ (or the transformation map

$T(x)$) would imply that the state estimate $\hat{x}$ asymptotically approaches the actual state x.

To ensure the feasibility and viability of the observer design (9), a set of necessary and sufficient conditions needs to be derived, under which the associated system of PDEs (11) admits a unique and invertible solution. Please notice, that in this case the proposed nonlinear observer (9) would exhibit the desirable convergence properties, or equivalently, it would generate state estimates that asymptotically converge to the actual unmeasurable states. Furthermore, and from a practical point of view, the use of the observer (9) requires the development of a comprehensive solution method for the system of PDEs (11). First, attention should be drawn to the fact that the above system of first-order PDEs is of particular structure and admits a common principal part that consists of the components $f_i(x)$, $(i = 1, \ldots, S+1)$ of the vector function $f(x)$ [38]. Furthermore, notice that the principal part vanishes at $x = 0$ due to the equilibrium condition, and thus, the origin becomes a characteristic (singular) point for the system of PDEs (11) [38]. As a consequence, the well-known existence and uniqueness Cauchy–Kovalevskaya theorem can not be invoked because the pertinent conditions are not satisfied for the singular system of PDEs (11) [38], and inevitably one needs to resort to methods and results from singular PDE theory. However, it can be proven that under a set of rather generic necessary and sufficient conditions the above system of singular PDEs (11) admits a unique locally analytic and invertible solution in the neighborhood of the reference equilibrium point $x = 0$ (Appendix; for detailed proofs please see [37]).

Let us now consider the problem of the development of a solution method for the system of PDEs (11). We would first like to point out, that the method of characteristics for the system of first-order PDEs (11) cannot be applied due to the singularity at the reference equilibrium point. However, as previously mentioned, the functions $f(x)$, $h(x)$, as well as the solution $T(x)$ are all locally analytic. Therefore, the proposed solution method is based on a multivariate Taylor series expansion of $f(x)$, $h(x)$ and the unknown solution $T(x)$, followed by a procedure that equates the Taylor coefficients of both sides of the system of PDEs (11). As a result, recursion algebraic formulas are generated that are linear with respect to the Taylor coefficients of the unknown solution, and in particular, one can calculate the N-th order Taylor coefficients of $T(x)$, given the Taylor coefficients of $T(x)$ up to the order $N-1$ already calculated in previous recursive steps. The above linear recursive formulas admit a compact mathematical represenation if tensorial notation is used. In particular, the same notational rules established in [37] will be considered:

(a) The entries of a constant matrix A are represented as a_i^j, where the subscript i refers to the corresponding row and the superscript j to the corresponding column of the matrix.

(b) The partial derivatives of the μ component $f_\mu(x)$ of a vector field $f(x)$ at $x = 0$ are denoted as follows:

$$f_\mu^i = \frac{\partial f_\mu}{\partial x_i}(0), \qquad f_\mu^{ij} = \frac{\partial^2 f_\mu}{\partial x_i\, \partial x_j}(0), \qquad f_\mu^{ijk} = \frac{\partial^3 f_\mu}{\partial x_i\, \partial x_j\, \partial x_k}(0),$$

etc.

(c) The widely-used summation convention is considered, according to which repeated upper and lower tensorial indices are summed up.

Please notice, that under the above notational convention, the l-th component $T_l(x)$ of the unknown solution $T(x)$ of the system of PDEs (11) can be represented in a multivariate Taylor series form in the following fashion:

$$T_l(x) = \frac{1}{1!} T_l^{i_1} x_{i_1} + \frac{1}{2!} T_l^{i_1 i_2} x_{i_1} x_{i_2} + \cdots + \frac{1}{N!} T_l^{i_1 i_2 \ldots i_N} x_{i_1} x_{i_2} \ldots x_{i_N} + \cdots \tag{13}$$

Similarly functions $f(x)$, $h(x)$ are expanded in Taylor series, and then inserted into PDEs (11). The next step, involves the procedure of matching the Taylor coefficients of the same order, that eventually leads to the following formula for the N-th order Taylor coefficients of the unknown solution $T(x)$ [37]:

$$\sum_{L=0}^{N-1} \sum_{\binom{N}{L}} T_l^{\mu i_1 \ldots i_L} f_\mu^{i_{L+1} \ldots i_N} = a_l^\mu T_\mu^{i_1 \ldots i_N} + b_l^\mu h_\mu^{i_1 \ldots i_N} \tag{14}$$

with $i_1, \ldots, i_N = 1, \ldots, S+1$ and $l = 1, \ldots, S+1$. Please notice, that the second summation symbol in (14) requires summing up the relevant quantities over the $\binom{N}{L}$ possible combinations of the indices $(i_1, \ldots, i_N)$. As mentioned earlier, equations (14) represent a set of linear algebraic equations with respect to the unknown coefficients $T_\mu^{i_1, \ldots, i_N}$. This is precisely the mathematical reason, that allows the proposed series solution method for the system of singular PDEs (11) to be easily implemented through a symbolic software package such as MAPLE. Indeed, a simple MAPLE code has been developed that automatically calculates the various higher-order Taylor coefficients of the unknown solution of (11).

Remark 1. The proposed state observer (9) is based on the explicit construction of an invariant manifold map $z = T(x)$ for the augmented system:

$$\begin{aligned} \frac{\mathrm{d}x(t)}{\mathrm{d}t} &= f(x(t)), \\ \frac{\mathrm{d}z(t)}{\mathrm{d}t} &= Az(t) + Bh(x(t)), \end{aligned} \tag{15}$$

comprised of the original nominal dynamical system (7) and the observer dynamics expressed in the transformed coordinates. Indeed, it is easy to show

that the invariance requirement is mathematically translated into the system of invariance PDEs (11) that the map $z = T(x)$ ought to satisfy [10,34–36,39,40]. Finally, it should be pointed out, that the augmented system (15) falls within the class of the so-called skew-product systems [41], where the driving system represents the original system dynamics that drives (through the sensor measurements $y(t) = h(x(t))$) the state observer dynamics as shown in (15).

Remark 2. Under the assumptions stated, and in the linear case, where $f(x) = Fx$ and $h(x) = Hx$, the associated system of singular PDEs (11) admits a unique solution: $T(x) = \mathcal{T}x$, with $\mathcal{T}$ being the invertible unique solution of the Sylvester-type matrix equation [14,42]: $\mathcal{T}F - A\mathcal{T} = BH$. In this case, the proposed observer has a constant gain: $L = \mathcal{T}^{-1}b$, and coincides with the standard Luenberger observer [17].

Let us now examine the convergence properties of the state observer (9) in the presence of the model uncertainty or modeling error $g(x)$. From a mathematical point of view, we would like to investigate the possibility of the estimation error dynamics induced by the proposed observer (9) to be structurally stable in the presence of model uncertainty $g(x)$. Indeed, as shown earlier, observer (9) which was designed on the basis of the fully "known" nominal model (7) induces estimation error dynamics with assignable rate of decay described by (12). However, when model uncertainty $g(x)$ is taken into account the estimation error dynamics in the transformed coordinates: $e_z = z - \hat{z} = T(x) - T(\hat{x})$ becomes

$$\begin{aligned}\frac{\mathrm{d}e_z}{\mathrm{d}t} &= \frac{\partial T}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\partial T}{\partial \hat{x}}\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} \\ &= \frac{\partial T}{\partial x}\{f(x) + \epsilon g(x)\} - \frac{\partial T}{\partial \hat{x}}\{f(\hat{x}) + L(\hat{x})(y - h(\hat{x}))\} \\ &= AT(x) + Bh(x) + \varepsilon\frac{\partial T}{\partial x}g(x) - AT(\hat{x}) - Bh(\hat{x}) - Bh(x) + Bh(\hat{x}) \\ &= Ae_z + \epsilon\frac{\partial T}{\partial x}(x)g(x). \end{aligned} \tag{16}$$

Please notice that the above error dynamics is not linear anymore due to model uncertainty and the presence of the nonlinear term $\varepsilon(\partial T/\partial x)(x)g(x)$. In particular, it can be mathematically characterized as a perturbed dynamical system comprised of a nominal linear dynamical system with a stable fundamental matrix A induced by the design of the state observer (9), and a perturbation term $\varepsilon(\partial T/\partial x)g(x)$. Equation (16) yields [43]:

$$e_z(t) = \exp(At)e_z(0) + \int_0^t \exp(A(t-\tau))\left[\varepsilon\frac{\partial T}{\partial x}(x(\tau))g(x(\tau))\right]d\tau \tag{17}$$

Furthermore, since A has stable eigenvalues (Hurwitz matrix), there exist positive constants $\beta > 0$, $\gamma > 0$ such that [42,43]:

$$||\exp(At)|| \leqslant \gamma\ \exp(-\beta t). \tag{18}$$

In light of inequality (18), the following bound on the estimation error can be established:

$$
\begin{aligned}
||e_z(t)|| &\leqslant ||\exp(At)||||e_z(0)|| + \int_0^t ||\exp(A(t-\tau))|| \left\{\epsilon||\frac{\partial T}{\partial x}(x(\tau))||||g(x(\tau))||\right\} \mathrm{d}\tau \\
&\leqslant \gamma \exp(-\beta t)||e_z(0)|| + \gamma\epsilon LM \int_0^t \exp(-\beta(t-\tau))\,\mathrm{d}\tau \\
&\leqslant \gamma \exp(-\beta t)||e_z(0)|| + \epsilon\frac{\gamma LM}{\beta}(1-\exp(-\beta t)) \\
&= \gamma||e_z(0)||\exp(-\beta t) - \epsilon\frac{\gamma LM}{\beta}\exp(-\beta t) + \epsilon\frac{\gamma LM}{\beta},
\end{aligned} \tag{19}
$$

where $e_z(0)$ is the initial estimation error of the unmeasurable states and $||\partial T/\partial x|| \leqslant L$ in the compact set X. On the basis of result (19) the following important remarks can be made:

(i) In the absence of model uncertainty/modeling error: $g(x) \equiv 0$, the estimation error in the transformed coordinates decays to zero: $||e_z(t)|| = ||\hat{z}(t) - z(t)|| = ||T(\hat{x}(t)) - T(x(t))|| \longrightarrow 0$, as $t \longrightarrow \infty$. Invoking the analyticity and local invertibility property of the coordinate transformation map $z = T(x)$, one readily establishes convergence of the estimation error expressed in the original coordinates: $||e(t)|| = ||\hat{x} - x|| \longrightarrow 0$, as $t \longrightarrow \infty$.

(ii) Notice that due to the presence of the model uncertainty term $g(x)$ the estimation error does not converge asymptotically to zero even in the presence of zero initial estimation error: $e_z(0) = 0$. However, as can be easily inferred from (19), the inevitable offset is of order $O(\epsilon)$. Equivalently stated, the estimation error will be ultimately bounded by a small bound if the perturbation/model uncertainty term is itself bounded by a small bound. In particular, inequality (19) derived for the bound of the estimation error suggests that it is directly proportional to the magnitude of the model uncertainty term.

Within the context of the present study, the issue of time-varying process parameters or model inputs (such as catalyst deactivation, enzymatic degradation, certain types of model uncertainty associated with the values of kinetic rate constants, etc.) appearing in the dynamic equations of the nominal system (7) can be addressed as well. Indeed, this type of situation is frequently encountered in practice and is mathematically realized by the following state-space representation for the nominal nonlinear (bio)chemical reaction system [1,3,28,32,43]:

$$
\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t} &= f(x) = f_0(x) + f_1(x, u(t)), \\
y &= h(x),
\end{aligned} \tag{20}
$$

where $u \in R^p$ is now the vector of the time-varying model input variables, $f_0 : R^{S+1} \longrightarrow R^{S+1}$, $f_1 : R^{S+1} \times R^p \longrightarrow R^{S+1}$ are real analytic vector functions in the domain X, with $L(u)$ being a Lipschitz constant for f_1 on X. The first step in our analysis is to ensure asymptotic stability of the estimation error dynamics (as the state estimate converges to the actual state) for the nominal system (20) in the presence of the time-varying model input variables $u(t)$. Please notice, that once asymptotic stability is established for the nominal input-driven system (20), taking into account and integrating into the analysis framework the perturbatory model uncertainty term $\epsilon g(x)$ as well:

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= f(x) + \epsilon g(x) = f_0(x) + f_1(x, u(t)) + \epsilon g(x), \\ y &= h(x), \end{aligned} \tag{21}$$

becomes quite straightforward by following exactly the same methodological steps outlined earlier and omitted here for brevity. Therefore, in light of the above remark, the focus is now placed on the stability (convergence) properties of the estimation error dynamics induced in this case by the following state observer:

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = f_0(\hat{x}(t)) + f_1(\hat{x}(t), u(t)) + L(\hat{x}(t))(y(t) - h(\hat{x})(t)), \tag{22}$$

where the observer gain is given by

$$L(x) = \left[\frac{\partial T}{\partial x}(x)\right]^{-1} B,$$

with $T(x)$ being the solution of the system of singular PDEs (11). Indeed, the above observer gives rise to the following estimation error $e_z = z - \hat{z} = T(x) - T(\hat{x})$ dynamics:

$$\begin{aligned} \frac{de_z}{dt} = &-\frac{\partial T}{\partial \hat{x}} \left\{ f_0(\hat{x}) + f_1(\hat{x}, u) + \left[\frac{\partial T}{\partial \hat{x}}(\hat{x})\right]^{-1} B(y - h(\hat{x})) \right\} \\ &+ \frac{\partial T}{\partial x}(f_0(x) + f_1(x, u)) = Ae_z + \Omega(x, u) - \Omega(\hat{x}, u), \end{aligned} \tag{23}$$

where $\Omega(x, u) = (\partial T / \partial x)(x) f_1(x, u)$. Consider now the quadratic function:

$$V(e_z) = e_z^T P e_z, \tag{24}$$

where P is the unique positive-definite solution to the following Lyapunov matrix equation [14]:

$$A^T P + PA = -2Q \tag{25}$$

with A being Hurwitz and Q an arbitrarily selected positive-definite matrix. Let us now calculate the time-derivative of the above quadratic function along the trajectories of the error dynamics (24):

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}t} &= \left(\frac{\mathrm{d}e_z}{\mathrm{d}t}\right)^T Pe_z + e_z^T P\frac{\mathrm{d}e_z}{\mathrm{d}t} \\ &= e_z^T(A^T P + PA)e_z + 2e_z^T P[\Omega(x,u) - \Omega(\hat{x},u)] \\ &= -2e_z^T Qe_z + 2e_z^T P[\Omega(\hat{x}+e,u) - \Omega(\hat{x},u)].\end{aligned} \tag{26}$$

From (27) one easily obtains:

$$\frac{\mathrm{d}V}{\mathrm{d}t} \leqslant -2e_z^T Qe_z + 2L(u)||P||||e||||e_z||, \tag{27}$$

where $e = x - \hat{x}$ is the estimation error expressed in the original coordinate system. Invoking the local analyticity and invertibility of $T(x)$ in the compact domain X, it is inferred that there exists a positive number δ such that: $||e|| \leqslant \delta||e_z||$, and therefore equation (28) yields:

$$\frac{\mathrm{d}V}{\mathrm{d}t} \leqslant -2e_z^T Qe_z + 2\delta L(u)||P||||e_z||^2. \tag{28}$$

Notice, that the norm of the symmetric positive-definite matrix P is given by [44]:

$$||P|| = \lambda_{\max}(P), \tag{29}$$

where $\lambda_{\max}(P)$ is the maximum eigenvalue of matrix P, and for the positive-definite matrix Q the following inequality holds [44]:

$$e_z^T Qe_z \geqslant \lambda_{\min}(Q)||e_z||^2, \tag{30}$$

where $\lambda_{\min}(Q)$ is the minimum eigenvalue of matrix Q. In light of equations (29) and (30), one now obtains

$$\frac{\mathrm{d}V}{\mathrm{d}t} \leqslant (-2\lambda_{\min}(Q) + 2L(u)\delta\lambda_{\max}(P))||e_z||^2. \tag{31}$$

Therefore, if matrix Q is selected such that

$$\frac{\lambda_{\min}(Q)}{\lambda_{\max}(P)} > L(u)\delta \tag{32}$$

the time-derivative of the positive-definite quadratic function (25) becomes negative, the function $V(e)$ qualifies as a Lyapunov function for the estimation error dynamics (24), and therefore, by invoking Lyapunov's theorem [43], asymptotic stability of the estimation error dynamics (24) is readily established.

The above results suggest that the proposed state observer is capable of providing accurate and robust estimates of the unmeasurable state variables in the presence of suitably modeled and rather broad classes of modeling errors/model uncertainties. The performance, convergence properties and robustness of the proposed observer will be evaluated in the next section's illustrative case study.

4. Illustrative example: A nonlinear biochemical reaction system

A biochemical reaction system is considered where cells are being grown through the consumption of a substrate in a typical continuous stirred-tank biological reactor [4,7]. In particular, under the assumption of constant volume, the following dynamic model can be obtained [4,7]:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}t} &= \mu(X, S)X - \frac{F}{V}X, \\ \frac{\mathrm{d}S}{\mathrm{d}t} &= -\frac{\mu(X, S)X}{Y} + \frac{F}{V}(S_F - S), \end{aligned} \tag{33}$$

where X, S are the cell-mass and substrate concentrations respectively, $\mu(X, S)$ the specific growth rate, Y the yield coefficient, F the feedrate of the substrate, S_F the feed concentration and V the reactor volume. Under the assumption of Contois kinetics the specific growth rate assumes the following form [7]:

$$\mu(X, S) = \frac{K_1 S}{K_2 X + S}, \tag{34}$$

where K_1, K_2 are kinetic constants, and thus, the dynamic model (33) takes the form:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}t} &= \frac{K_1 X S}{K_2 X + S} - \frac{F}{V}X, \\ \frac{\mathrm{d}s}{\mathrm{d}t} &= -\frac{K_1 X S}{Y(K_2 X + S)} + \frac{F}{V}(S_F - S). \end{aligned} \tag{35}$$

The following values are assigned to the model parameters: $K_1 = 1\ (\mathrm{min}^{-1})$, $K_2 = 1$, $Y = 1$, $F/V = 0.08\ (\mathrm{min}^{-1})$, $S_F = 0.1\ (\mathrm{kg\,m}^{-3})$. Moreover, notice that in this case the equilibrium point is: $(X^0, S^0) = (0.092, 0.008)$. Let us now assume that the value of the K_1 kinetic constant is not fully known, but uncertain. It is assumed that: $K_1 = K_1^0 + \epsilon \sin(t)$, where $K_1^0 = 1\ (\mathrm{min}^{-1})$ is a known nominal value and $\epsilon \sin(t)$ represents a bounded time-varying term reflecting the uncertainty that characterizes the numerical value of K_1, with $\epsilon > 0$ being a small positive constant. Given the structure of the above dynamic model (35) and denoting the state variables by $x_1 = X > 0, x_2 = S > 0$, it can be easily deduced that the perturbation term is given

by the following expression:

$$g(x_1, x_2) = \begin{bmatrix} \frac{\sin(t)\, x_1 x_2}{x_1 + x_2} \\ \frac{-\sin(t)\, x_1 x_2}{x_1 + x_2} \end{bmatrix}. \tag{36}$$

Furthermore, it can be easily proven that the nominal system is asymptotically stable around the equilibrium point of interest (through a simple calculation of the eigenvalues of the Jacobian matrix associated with the linearized system around the equilibrium point), and standard Lyapunov techniques can offer an estimate of the stability region and a compact set in state space: $X = \{x = (x_1, x_2) \in R^2 : ||x|| = \sqrt{x_1^2 + x_2^2} < r\}$ within which the system's trajectory remains confined (the radius r depends of course on the initial conditions: $||x(0)|| < l$) [43]. Therefore, one obtains the following bound for $g(x)$:

$$\begin{aligned} ||g(x)|| = ||g(x_1, x_2)|| &= \sqrt{2}\frac{|\sin(t)| x_1 x_2}{x_1 + x_2} \\ &\leqslant \sqrt{2}\frac{x_1 x_2}{x_1 + x_2} \leqslant \sqrt{2} x_1 \\ &\leqslant \sqrt{2}\sqrt{x_1^2 + x_2^2} = \sqrt{2}||x|| < \sqrt{2} r = M \end{aligned} \tag{37}$$

for $||x|| < r$.

The objective is to estimate the unmeasured substrate concentration $\hat{x_2}(t)$, by using on-line measurements of the cell-mass concentration $y(t) = h(x(t)) = x_1(t)$ [44] in the presence of model uncertainty $g(x)$ considered above. In order to accomplish the task of estimating $\hat{x_2}(t)$, the nonlinear state observer (9) is proposed. According to the methodology developed in Section 3, the following system of first-order singular PDEs needs to be solved first:

$$\begin{aligned} &\frac{\partial w_1}{\partial x_1}\left(\frac{x_1 x_2}{x_1 + x_2} - 0.08 x_1\right) + \frac{\partial w_1}{\partial x_2}\left(-\frac{x_1 x_2}{x_1 + x_2} - 0.08 x_2 + 0.008\right) \\ &\quad = a_{11} w_1 + a_{12} w_2 + b_1 x_1, \\ &\frac{\partial w_2}{\partial x_1}\left(\frac{x_1 x_2}{x_1 + x_2} - 0.08 x_1\right) + \frac{\partial w_2}{\partial x_2}\left(-\frac{x_1 x_2}{x_1 + x_2} - 0.08 x_2 + 0.008\right) \\ &\quad = a_{21} w_1 + a_{22} w_2 + b_2 x_1, \\ &\qquad w_1\left(x_1^0, x_2^0\right) = w_1(0.092, 0.008) = 0, \\ &\qquad w_2\left(x_1^0, x_2^0\right) = w_2(0.092, 0.008) = 0. \end{aligned} \tag{38}$$

The following parameters have been selected for matrices $\{A, B\}$:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} -0.1 & 0 \\ 0 & -0.2 \end{bmatrix}, \tag{39}$$

and

$$B = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}. \tag{40}$$

Under the above choice of design parameters the system of singular PDEs (38) admits a unique locally analytic and invertible solution $T(x)$. A series solution of the above system of PDEs (38) is then sought around the equilibrium point of interest $(x_1^0, x_2^0) = (0.092, 0.008)$. The Taylor coefficients of the unknown solution $T(x_1, x_2)$ are automatically computed by using a simple MAPLE code. In particular, a third-order truncation $T^{[3]}(x_1, x_2)$ of the Taylor series expansion of $T(x_1, x_2)$ is considered and given by

$$\begin{aligned} T_1^{[3]}(x_1, x_2) = {} & 10.1224(x_1 - 0.092) - 1.6887(x_2 - 0.008) \\ & + 0.1254(x_1 - 0.092)^2 - 3.4561(x_1 - 0.092)(x_2 - 0.008) \\ & + 29.8104(x_2 - 0.008)^2 - 1.2314(x_1 - 0.092)^3 \\ & + 32.0972(x_1 - 0.092)^2(x_2 - 0.008) \\ & - 191.0671(x_1 - 0.092)(x_2 - 0.008)^2 \\ & - 399.6450(x_2 - 0.008)^3 \\ & + \mathcal{O}(|x_1 - 0.092|^4, |x_2 - 0.008|^4) \end{aligned} \tag{41}$$

and

$$\begin{aligned} T_2^{[3]}(x_1, x_2) = {} & 10.0613(x_1 - 0.092) - 0.7690(x_2 - 0.008) \\ & + 0.0572(x_1 - 0.092)^2 - 1.4475(x_1 - 0.092)(x_2 - 0.008) \\ & + 9.1546(x_2 - 0.008)^2 - 1.7181(x_1 - 0.092)^3 \\ & + 13.6812(x_1 - 0.092)^2(x_2 - 0.008) \\ & - 73.4817(x_1 - 0.092)(x_2 - 0.008)^2 \\ & - 110.8042(x_2 - 0.008)^3 \\ & + \mathcal{O}(|x_1 - 0.092|^4, |x_2 - 0.008|^4). \end{aligned} \tag{42}$$

On the basis of the above third-order polynomial approximation $T^{[3]}(x_1, x_2)$ of the actual solution $T(x)$ of (38) the proposed nonlinear observer (9) was simulated for different values of ϵ in order to obtain estimates of the unmeasurable state variable $x_2(t) = S(t)$ (figures 1–3). In particular, figure 1 depicts the actual state $S(t)$ and its estimate for a value of $\epsilon = 0.1$, showing the satisfactory convergence properties of the proposed observer, as the state estimate converges nicely to the actual substrate concentration profile. The value of ϵ is then increased to $\epsilon = 0.3$ for the simulation results shown in figure 2. As was theoretically predicted in earlier sections, the impact of a greater uncertainty associated with the numerical value of the kinetic constant K_1 on the convergence properties of the proposed observer is now becoming more visible. However, convergence of

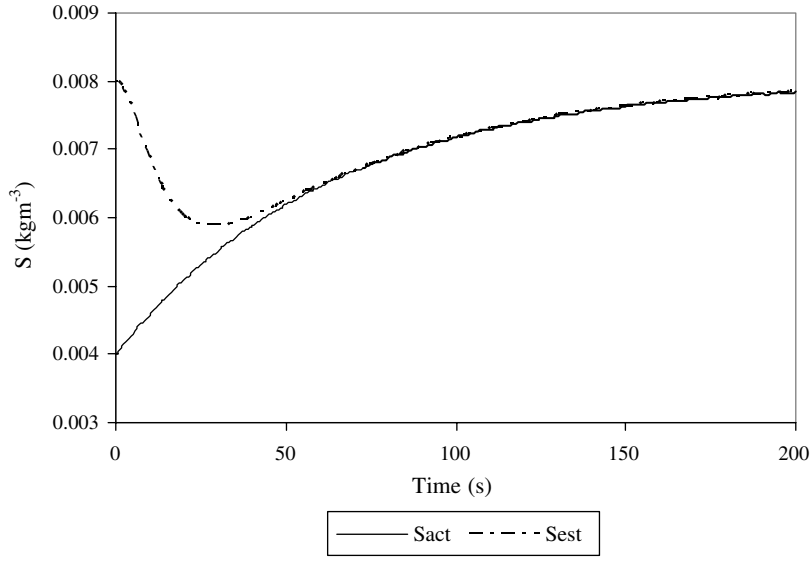

Figure 1. Estimation of substrate concentration for $\epsilon = 0.1$.

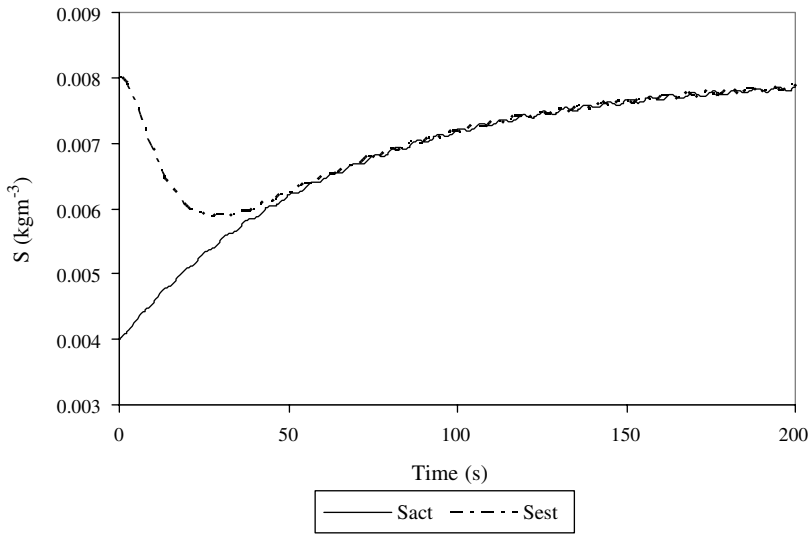

Figure 2. Estimation of substrate concentration for $\epsilon = 0.3$.

the observer's state estimate to the actual process state $S(t)$ remains still fairly good. In figure 3 simulation results are shown for a higher degree of uncertainty on K_1 and for a value of $\epsilon = 0.9$. Pleasse notice, that the impact of the model uncertainty is now substantial, performance deterioration of the observer (9) as indicated in the above theoretical investigations becomes noticeable, leading to

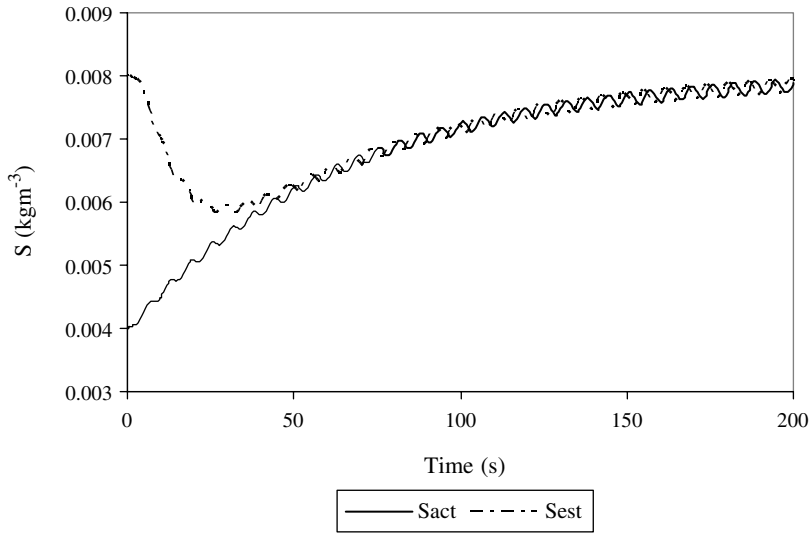

Figure 3. Estimation of substrate concentration for $\epsilon = 0.9$.

an apparent offset between the observer's state estimate and the actual substrate concentration profile.

5. Concluding remarks

In the present study a new approach to the unmeasurable state reconstruction problem for nonlinear chemical reaction systems in the presence of model uncertainty is proposed. The proposed nonlinear state observer possesses a state-dependent gain which is computed from the solution of a system of first-order singular partial differential equations (PDEs). Furthermore, a set of conditions is provided that ensure the existence and uniqueness of a locally analytic and invertible solution to the aforementioned system of singular PDEs, and a series solution method is developed that can be easily implemented through a MAPLE code. Under these conditions, the convergence of the estimation error to zero is analyzed in the presence of model uncertainty. Finally, the performance of the proposed state observer was evaluated in an illustrative biochemical reaction system.

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A. Appendix: Existence and uniqueness conditions for the solution of the system of singular PDEs (11)

Under the following set of conditions, the system of first-order singular PDEs (11) admits a unique locally analytic and invertible solution $z = T(x)$ in a neighborhood of the origin [37]:

Condition 1. The Jacobian matrix F has eigenvalues $k_i (i = 1, \ldots, S+1)$ with

$$0 \notin co\{k_1, k_2, \ldots, k_{S+1}\}, \tag{43}$$

where *co* stands for the convex hull of a set. Equivalently stated, the spectrum of F belongs to the Poincaré domain [45]. It should be pointed out, that this assumption has been recently relaxed in [28], where existence and uniqueness of a solution to the system of PDEs (11) is proved under the rather generic assumption that the spectrum of F lies wholly in the Siegel domain [28,45].

Condition 2. The following $(m(S+1)) \times (S+1)$ matrix O:

$$O = \begin{bmatrix} H \\ HF \\ \vdots \\ HF^S \end{bmatrix} \tag{44}$$

has rank $S+1$.

Condition 3. The following $(S+1) \times (m(S+1))$ matrix $\mathcal{C}$:

$$\mathcal{C} = \begin{bmatrix} B & AB & \ldots & A^S B \end{bmatrix} \tag{45}$$

has rank $S+1$. It can be shown that Conditions 2 and 3 are crucial in order to ensure local invertibility of the unknown solution $T(x)$ of (11) [37].

Condition 4. The eigenvalues $k_i, (i = 1, \ldots, S+1)$ of F are not related to the eigenvalues $\lambda_i, (i = 1, \ldots, S+1)$ of A through any equation of the type:

$$\sum_{i=1}^{S+1} m_i k_i = \lambda_j \tag{46}$$

($j = 1, \ldots, S+1$), where all the m_i are non-negative integers that satisfy the condition:

$$\sum_{i=1}^{S+1} m_i > 0. \tag{47}$$

Conditions 1 and 4 are necessary for the existence and uniqueness of the unknown solution $T(x)$ of (11). In particular, Condition 1 ensures the uniform convergence of the formal power series representation of the unique solution $T(x)$, and hence, its analyticity property [37].

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