Digital Control and Monitoring Methods for Nonlinear Processes

A Thesis
Presented to
The Academic Faculty

by

Nguyen Huynh

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy

Chemical Engineering
Worcester Polytechnic Institute
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ABSTRACT

The chemical engineering literature is dominated by physical and (bio)-chemical processes that exhibit complex nonlinear behavior, and as a consequence, the associated requirements of their analysis, optimization, control and monitoring pose considerable challenges in the face of emerging competitive pressures on the chemical, petrochemical and pharmaceutical industries. The above operational requirements are now increasingly imposed on processes that exhibit inherently nonlinear behavior over a wide range of operating conditions, rendering the employment of linear process control and monitoring methods rather inadequate. At the same time, increased research efforts are now concentrated on the development of new process control and supervisory systems that could be digitally implemented with the aid of powerful computer software codes. In particular, it is widely recognized that the important objective of process performance reliability can be met through a comprehensive framework for process control and monitoring. From:

(i) a process safety point of view, the more reliable the process control and monitoring scheme employed and the earlier the detection of an operationally hazardous problem, the greater the intervening power of the process engineering team to correct it and restore operational order

(ii) a product quality point of view, the earlier detection of an operational problem might prevent the unnecessary production of off-spec products, and subsequently minimize cost.

The present work proposes a new methodological perspective and a novel set of systematic analytical tools aiming at the synthesis and tuning of well-performing digital controllers and the development of monitoring algorithms for nonlinear processes. In particular, the main thematic and research axis traced are:

(i) The systematic integrated synthesis and tuning of advanced model-based digital controllers using techniques conceptually inspired by Zubov's advanced stability theory.

(ii) The rigorous quantitative characterization and monitoring of the asymptotic behavior of complex nonlinear processes using the notion of invariant manifolds and functional equations theory.

(iii) The systematic design of nonlinear state observer-based process monitoring systems to accurately reconstruct unmeasurable process variables in the presence of time-scale multiplicity.

(iv) The design of robust nonlinear digital observers for chemical reaction systems in the presence of model uncertainty.

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CHAPTER 1

Parametric Optimization of Digitally Controlled Nonlinear Reactor Dynamics

1.1 Introduction

In recent years, the development of powerful analytical and computational tools enabled the analysis of the dynamic behavior of complex nonlinear chemical reaction systems to be performed in a thorough and rigorous manner [42, 43, 86, 95]. As a result, the "inverse problem" of modifying and controlling the above dynamic behavior has also received considerable attention [18, 28]. In particular, it is widely recognized that quite often the chemical reactor dynamics is often driven by "input" variables associated with the reactor feeding and reaction initiation policy (feed flow rates, reactant inlet concentration, etc.), and therefore it is amenable to modification through feedback action and the subsequent enforcement of the desirable dynamic modes and behavior [18, 28]. Equivalently stated, one may derive a feedback control law that dictates the appropriate input profile, which in turn, enforces the requisite and desirable dynamic behavior on the controlled reactor dynamics. In particular, unexpected disturbances may occur driving the chemical reactor far from the design steady state conditions, and the primary objective is to derive a control law capable

of driving the system back to the design steady-state in a smooth, fast and reliable manner, thus rejecting the disturbance effect [18, 28].

The above represents a typical scenario of a reactor regulation problem that can be adequately addressed via the action of a feedback controller. Please notice, that a feedback regulator enjoys design flexibility by introducing tunable controller parameters that can be adjusted in order to assign the desirable dynamic characteristics to the controlled reactor dynamics (speed and non-oscillatory characteristics of the reactor's response, tolerable overshoot, size of the stability region, transient behavior towards the stable manifold, as well as other asymptotic properties) [18, 48].

Over the last two decades significant research effort has concentrated on the nonlinear feedback controller synthesis problem, in order to overcome performance limitations associated with linear controller design methods applied to linearized reactor dynamic models [18,48]. Furthermore, the advent of digital technology revolutionized the way advanced nonlinear feedback control algorithms are implemented in practice with the aid of a computer. Nowadays, computer-based digital control systems are successfully designed and used in a multitude of applications [57, 78]. However, the problem of systematically selecting the digital controller parameters for nonlinear chemical reactors has not been given proper attention, and has been traditionally addressed either through heuristics or trial-and-error type of approaches, thus inevitably resorting to extensive dynamic simulations and/or costly experiments [51,78]. The proposed approach aims at the development of a systematic and comprehensive method to optimally select the parameters of a nonlinear digital reactor control system, when in addition to standard performance requirements of the controlled reactor dynamics (stability, fast and smooth regulatory response and disturbance rejection), optimality is also requested with respect to a physically meaningful performance index.

In the present study [47], the tunable parameters of the feedback controlled reactor dynamics are optimally selected through the minimization of a performance index, representing the decision variables of the associated optimization problem. Under this formulation, the problem under consideration becomes a finite-dimensional static optimization problem, as opposed to an infinite-dimensional nonlinear optimal control problem that could exhibit computational challenges in practice [10]. Traditionally, the above optimization problem is carried out in a "brute force" manner: after an initial guess for the controller parameters, the dynamic equations of the controlled reactor dynamics are simulated and the value of the performance functional is calculated numerically. Then, a gradient-direction method is typically applied to update the controller parameter values until convergence of the recursive algorithm leads to an optimal set of controller parameter values [10]. More elaborate methods from an algorithmic and computational point of view have also appeared in the pertinent body of literature. They rely either on numerical techniques for solving challenging two-point boundary value problems, or large scale nonlinear mathematical programs resulting from time-discretization and parameterization of the input variables [10,31].

The present research study introduces a systematic and practical methodology that addresses the above finite-dimensional static parametric optimization problem for digitally controlled nonlinear reactor dynamics. In particular, the proposed approach is based on the explicit calculation of a physically meaningful quadratic performance index by solving a Zubov-like functional equation. It can be proven that the functional equation admits a unique locally analytic solution in the vicinity of the reference equilibrium point, which is also endowed with all the properties of a Lyapunov function for the controlled reactor dynamics. Therefore, a transparent and very useful link between optimality and stability can be established through the solution of the above functional equation. Furthermore, the analyticity of the solution enables the development of a series solution method for the functional equation that can be

easily implemented with the aid of a symbolic software package such as MAPLE. It is also shown that the evaluation of the above Lyapunov function solution at the initial conditions leads to an explicit calculation of the value of the performance index. Since the dynamic equations of the controlled reactor dynamics are parameterized by the controller parameters, the Lyapunov function and solution to the functional equation is also parameterized, and therefore, the value of the performance index depends explicitly on the controller parameters. In light of the above observation, the employment of static optimization techniques can provide the optimal values of the finite set of controller parameters. Moreover, it should be pointed out, that for the optimally calculated controller parameter values, an explicit estimate of the size of the system's stability region can also be provided by using results from advanced stability theory for discrete dynamical systems [27, 80].

The present chapter is organized as follows: In Section 1.2 a succinct description of the requisite mathematical preliminaries and background is provided. Section 1.3 encompasses the main ideas and algorithmic structure of the proposed approach for parametric optimization of nonlinear digitally controlled reactor dynamics. In Section 1.4 simulation studies have been conducted in a representative chemical reactor example in order to evaluate the proposed method and illustrate its applicability. Finally, a few concluding remarks are provided in Section 1.5.

1.2 Mathematical Preliminaries and Motivation

Before we embark on the presentation of the proposed parametric optimization scheme for nonlinear digitally controlled reactor dynamics, let's first consider the simpler case of linear reactor dynamics in order to conceptually and methodologically motivate the development of its nonlinear analogue. The latter represents the focus of the present study. A linear (or linearized) autonomous dynamic system is considered

in the discrete-time domain:

$$x(k+1) = Ax(k) \tag{1.1}$$

where the non-negative integer $k \in \mathbb{N} = \{1, 2, ...\}$ is the discrete time index, $x(k) \in \mathbb{R}^n$ is the vector of state variables at the time instant k and A an $n \times n$ constant matrix. The above linear dynamic system in the discrete-time domain represents the linear discrete dynamics of a chemical reactor that is obtained either:

- through a reliable and accurate discretization method applied to the original continuous-time reactor dynamics in order to digitally (numerically) simulate the dynamic behavior of the reactor of interest [18, 52, 78]

or:

- through direct system identification methods and a set of historical input/output data, in the case where the reactor dynamics and the associated kinetics are discouragingly complex and not amenable to first-principle based modeling [18,78]. In both cases however, it is assumed that equation (1.1) adequately captures the actual linear reactor dynamics.

It is also assumed that the above system's characteristic matrix A has stable eigenvalues, which were assigned thanks to a fixed structure linear controller, designed in accordance to well-known methods [48, 78].

The following quadratic performance index associated with system (1.1) can be defined:

$$J = \sum_{k=0}^{\infty} [x(k)]^T Q [x(k)] \tag{1.2}$$

where Q is an arbitrarily selected positive-definite symmetric matrix, and the superscript T denotes the transpose of a vector or a matrix. Notice, that the aforementioned stability requirement on the reactor dynamics (1.1) implies that the infinite series in (1.2) converges to a fixed value limit [27, 80].

Introducing the following Lyapunov matrix equation:

$$A^T P A - P = Q \tag{1.3}$$

one can easily show that equation (1.3) admits a unique symmetric and positive-definite solution P [27]. Furthermore, applying standard Lyapunov stability theorems [27], it can be inferred that the quadratic form defined below:

$$V(x) = x^T P x \tag{1.4}$$

has the following properties:

$$\begin{gathered} V(x) > 0, V(0) = 0 \\ \Delta V(k) = V(x(k+1)) - V(x(k)) = -x(k)^T Q x(k) < 0 \end{gathered} \tag{1.5}$$

and therefore, it qualifies as a Lyapunov function [27]. Using equation (1.5) one obtains:

$$\begin{aligned} &J = \sum_{k=0}^{\infty} [x(k)]^T Q [x(k)] = -\sum_{k=0}^{\infty} V(x(k+1)) - V(x(k)) \\ &J = -(V(x(\infty))) - V(x(0)) = V(x(0)) \end{aligned} \tag{1.6}$$

since $V(x(\infty)) = V(x(k \to \infty)) = V(0) = 0$ due to the aforementioned stability assumption [27, 80].

Therefore, the value of the performance index J can be easily calculated through the formula below:

$$J = V(x(0)) = [x(0)]^T P [x(0)] \tag{1.7}$$

where P is the unique solution of the Lyapunov matrix equation (1.3) and $x(0)$ the initial value of the state vector. Please notice, that the interesting feature of this approach is signified by the underlying connection between optimality (performance index) and stability (Lyapunov function). This link was first explored and mathematically established by Bertram and Kalman [51] in the continuous time domain.

Let us now examine how the above ideas and techniques can be generalized in order to account for nonlinear reactor dynamics.

In particular, nonlinear reactor dynamics in the discrete time domain are considered:

$$x(k+1) = \varphi\left(x(k)\right) \tag{1.8}$$

where $x(k) \in \mathbb{R}^n$ is the vector of state variables at the discrete time instant k and $\varphi(x)$ a real analytic vector function defined on $\mathbb{R}^n$. Let x_0 be the reference (fixed) equilibrium point of interest:

$$\varphi(x_0) = x_0 \tag{1.9}$$

As it was mentioned in the linear reactor dynamics case, the discrete reactor dynamics and nonlinear difference equations (1.8) are assumed to have been obtained either through an accurate and reliable discretization method for the numerical (digital) simulation of the original continuous-time reactor dynamics, or through standard system identification methods [18, 48, 52, 57, 78]. It should be emphasized that the state space representation of the reactor dynamics (1.8) in the discrete time domain (realized via a nonlinear system of difference equations) represents the point of departure of any meaningful study of the digital reactor monitoring and control system design problem [78].

Furthermore, as in the linear case, let us assume that a fixed structure feedback controller has been designed, so that (1.8) represents the control reactor dynamics that has been rendered locally asymptotically stable. This is equivalent to assume that the Jacobian matrix of the linearized system $A = \dfrac{\partial \varphi}{\partial x}(x_0)$ has stable eigenvalues, i.e. eigenvalues that all lie inside the unit disc on the complex plane [78].

In this case, a quadratic performance index or cost function can be defined as follows:

$$J = \sum_{k=0}^{\infty} Q\left(x(k)\right) \tag{1.10}$$

where $Q(x)$ is an arbitrarily selected positive-definite real analytic scalar function defined on $\mathbb{R}^n$ with $Q(x_0)$ and $\dfrac{\partial Q}{\partial x}(x_0) = 0$.

Let us now introduce the following functional equation:

$$V\left(\varphi(x)\right) - V(x) = -Q(x) \tag{1.11}$$

accompanied by the boundary condition $V(x_0) = 0$ where the unknown solution is a scalar function $V(x)$ with $V\colon \mathbb{R}^n \to \mathbb{R}$. One easily observes:

$$J = \sum_{k=0}^{\infty} Q\left(x(k)\right) = -\sum_{k=0}^{\infty} \left[V\left(x(k+1)\right) - V\left(x(k)\right)\right] = V\left(x(0)\right) - V\left(\infty\right) \tag{1.12}$$

and since $V\left(x(\infty)\right) = V\left(x(k \to \infty) = V(x_0) = 0$ due to the stability assumption stated earlier, the following equality can be established:

$$J = V\left(x(0)\right) \tag{1.13}$$

Therefore, the above ideas allow a direct and explicit calculation of the value of the performance index in terms of the solution of the functional equation (1.11), assuming it exists and can be computed. Moreover, we are provided with some interesting properties concerning the solution $V(x)$ of the functional equation (1.11). Notice that by construction, the rate of change $\Delta V\left(x(k)\right)$ is negative definite since $Q(x)$ is positive definite:

$$\Delta V\left(x(k)\right) = V\left(\varphi\left(x(k)\right)\right) - V\left(x(k)\right) = -Q(x(k)) < 0 \tag{1.14}$$

and therefore, if the solution of the functional equation (1.11) can be proven to be positive definite, it also qualifies as a Lyapunov function for the controlled reactor dynamics (1.8) [27]. In such a case, the stability property of dynamics (1.8) and standard converse Lyapunov stability theorems for nonlinear discrete dynamical systems [27] imply the existence of a Lyapunov function that satisfies the functional equation (1.11). It should be emphasized, that the above construction represents exactly the discrete-time analogue of Zubov's PDE that was developed for the explicit computation of Lyapunov functions for nonlinear dynamical systems modeled through ODEs in the continuous-time domain [52, 80]. With respect to the above Zubov-like functional equation (1.11) the following important issues need to be addressed:

(i) **Existence and uniqueness of solution**

Theorems in references [55,56,60,80] guarantee the existence and uniqueness of a locally analytic solution $V(x)$ of the functional equation (1.11) in the vicinity of the reference equilibrium point x_0.

(ii) **Solution Method**

From a practical point of view, one needs to develop a comprehensive method for solving the functional equation (1.11). Since $\varphi(x)$, $Q(x)$ and the solution $V(x)$ are locally analytic, it is possible to calculate the solution $V(x)$ as a multivariate Taylor series around the equilibrium point of interest $x = x_0$. The proposed solution method can be realized through the following steps:

a. Expand $\varphi(x)$, $Q(x)$ and the unknown solution $V(x)$ in multivariate Taylor series and insert them into functional equation (1.11).

b. Equate the Taylor coefficients of the same order of both sides of functional equation (1.11)

c. Derive a hierarchy of linear recursion formulas through which one can calculate the N^{th} order coefficient of $V(x)$ given the Taylor coefficients up to order $N-1$ that have been computed in previous recursive steps.

It is feasible to explicitly derive the aforementioned recursive formulas and present them in a mathematically compact form if tensorial notation is used [60]:

a. The partial derivatives of the $\mu - th$ component $f_\mu(x)$ of a vector function $f(x)$ evaluated at $x = x_0$ are denoted as follows:

$$\begin{aligned} f_\mu^i &= \frac{\partial f_\mu}{\partial x_i}(x_0) \\ f_\mu^{ij} &= \frac{\partial^2 f_\mu}{\partial x_i \partial x_j}(x_0) \\ f_\mu^{ijk} &= \frac{\partial^3 f_\mu}{\partial x_i \partial x_j \partial x_k}(x_0), etc... \end{aligned} \tag{1.15}$$

b. The standard summation convention where repeated upper and lower tensorial indices are summed up.

Under the above notation, the unknown solution $V(x)$ of the functional equation (1.11) represented as a multivariate Taylor series attains the following form:

$$\begin{aligned} V(x) = \tfrac{1}{1!}V^{i_1}\left(x_{i_1} - x_{i_1,0}\right) + \tfrac{1}{2!}V^{i_1 i_2}\left(x_{i_1} - x_{i_1,0}\right)\left(x_{i_2} - x_{i_2,0}\right) + ... + \\ + \tfrac{1}{N!}V^{i_1 i_2 ... i_N}\left(x_{i_1} - x_{i_1,0}\right)...\left(x_{i_N} - x_{i_N,0}\right) + ... \end{aligned} \tag{1.16}$$

As mentioned above, one inserts the Taylor series expansions of $\varphi(x), Q(x), V(x)$ into functional equation (1.11) and starts equating coefficients of the same order. Since $Q(x_0) = \frac{\partial Q}{\partial x}(x_0) = 0$, one can easily show that $V(x)$ does not have linear terms in x: $\frac{\partial V}{\partial x} = 0$, or equivalently $V^{i_1} = 0$ for $i_1 = 1, ..., N$.

Furthermore, the following relation for the $N - th$ order coefficients can be obtained:

$$\sum_{L=1}^{N} \sum_{0 \le m_1 \le ... \le m_L} V^{j_1 ... j_L} \varphi_{j_1}^{m_1} ... \varphi_{j_L}^{m_L} = -Q^{i_1 ... i_N} \tag{1.17}$$

where $i_1, ..., i_N = 1, ..., n$, $m_1 + m_2 + ... + m_L = N$ and $N \ge 2$. Note that the second summation symbol in the above formula indicates summing up the relevant quantities over the $\frac{N!}{m_1!...m_L!}$ possible combinations to assign the N indices $(i_1, ..., i_N)$ as upper indices to the L positions $\varphi_{j_1}, ..., \varphi_{j_L}$, with m_1 of them being put in the first position, m_2 of them in the second one , etc $\left(\sum_{i=1}^{L} m_i = N\right)$ [60].

Please notice that the above expression represents a set of <u>linear</u> algebraic equations in the unknown coefficients $V^{i_1,...,i_N}$. This is precisely the mathematical reason that enables the proposed method to be easily implemented using a symbolic software package. Indeed, a simple and comprehensive MAPLE code has been developed to automatically compute the Taylor coefficients of the unknown solution $V(x)$ of the Zubov-like functional equation (1.11) (see Appendix A).

(iii) **Local positive definiteness of the solution** $V(x)$

Let:

$$\varphi(x) = x_0 + A(x - x_0) + \bar{\varphi}(x) \tag{1.18}$$

and:

$$Q(x) = (x - x_0)^T Q(x - x_0) + \bar{Q}(x) \tag{1.19}$$

with $\bar{\varphi}(x), \bar{Q}(x)$ real analytic and:

$$\bar{\varphi}(x_0) = \bar{Q}(x_0) = \frac{\partial \bar{\varphi}}{\partial x}(x_0) = \frac{\partial \bar{Q}}{\partial x}(x_0) = 0 \tag{1.20}$$

Furthermore, one may represent the solution $V(x)$ of (1.11) as follows:

$$V(x) = (x - x_0)^T P(x - x_0) + \bar{V}(x) \tag{1.21}$$

where:

$$\bar{V}(x_0) = \frac{\partial \bar{V}}{\partial x}(x_0) = \frac{\partial^2 \bar{V}}{\partial x^2}(x_0) = 0 \tag{1.22}$$

It can be easily shown that matrix P satisfies the following Lyapunov matrix equation:

$$A^T P A - P = -Q \tag{1.23}$$

which coincides with the one encountered in the linear case (Equation (1.3)). Under the assumptions stated, the above matrix equation admits a unique, positive-definite and symmetric solution P, and therefore, $V(x)$ is locally positive definite and a Lyapunov function for the controlled reactor dynamics (1.8) [27].

(iv) **Stability region estimates** $V(x)$

Let N be the truncation order corresponding to an N^{th}-order Taylor polynomial approximation $V^{(N)}(x)$ of the solution of the Zubov-like functional equation (1.11).

Let:

$$\Omega^N = \{x \in \mathbb{R}^n | x \neq x_0 \wedge \Delta V(x) = 0\} \tag{1.24}$$

and:

$$C^{(N)} = \min_{x \in \Omega^{(N)}} V^{(N)}(x) \tag{1.25}$$

Then, thanks to standard Lyapunov stability theorems for nonlinear discrete-time systems, the set $S^{(N)}(x)$ defined below can be proven to be wholly contained in the stability region of system (1.8) [27]:

$$S^{(N)}(x) = \left\{ x \in \mathbb{R}^n | V^{(N)}(x) \leq C^{(N)} \right\} \tag{1.26}$$

Therefore, the set $S^{(N)}$ represents an estimate of the system's stability region [27, 80].

1.3 The Proposed Approach

The link established in the previous section between optimality and reactor stability through a Lyapunov function satisfying a Zubov-like functional equation can adequately serve the purposes of optimally choosing the parameters of a digital control system with respect to a performance index. In particular, the optimal selection of the digital controller parameters can be attained through the static optimization of the performance index, whose value is explicitly calculated through the solution of the functional equation that is now parameterized by the controller parameters. Let us consider the following nonlinear discrete-time dynamical system with a state space representation describing the input-driven reactor dynamics:

$$x(k+1) = \varphi\left(x(k), u(k)\right) \tag{1.27}$$

where:

- $k = 0, 1, ...$ is the discrete time index
- $u \in \mathbb{R}$ is the input variable (typically being the feed flow rate, or the inlet reactant concentration, or the temperature of the feed stream, etc.) that can be manipulated according to a "control law" that modifies the reactor dynamics and enforces the desired dynamic behavior [18, 35, 48, 57]
- $x(k) \in \mathbb{R}^n$ is the vector of state variables

- $\varphi\left(x, u(x)\right)$ and $h(x)$ are real analytic functions defined on $\mathbb{R}^n \times \mathbb{R}$ and $\mathbb{R}^n$ respectively.

Without loss of generality, it is assumed that the origin $x_0 = 0$ is the reference equilibrium point that corresponds to: $u = u_0 = 0 : \varphi(0,0) = 0$.

A typical scenario of a reactor regulation problem presupposes that exogeneous disturbances unexpectedly occurred driving the system far from the design steady state conditions. The control objective is to derive a control law that would dictate the requisite pattern of manipulating the input variable , modify the reactor dynamics in a desirable fashion (the reactor dynamics is driven by u) and bring the system back to the design steady state, thus rejecting the effect of the disturbances. There is a variety of well-performing and carefully synthesized nonlinear reactor regulation laws in the pertinent body of literature [18, 48, 78], and the simplest of which exhibits the following structure:

$$u(k) = \kappa\left(x(k), p\right) \tag{1.28}$$

where $p \in P$ represents the m-dimensional vector of controller parameters and P the admissible parameter space, which is assumed to be a compact subset of $\mathbb{R}^m$. Furthermore, $\kappa\left(x; p\right)$ is assumed to be a real analytic scalar function, defined on $\mathbb{R}^n \times P$, with $\kappa\left(0; p\right) = 0$.

It should be pointed out, that all system regulation laws introduce a set of controller parameters $p \in P$ [18,48,78]. The latter reflect the controller degrees of freedom (the controller design flexibility). Indeed, the controller parameters are selected in such a manner that the desired dynamic behavior is assigned to the controlled reactor dynamics by the regulator. Desirable characteristics would be a stable, non-oscillatory and relatively fast response/reversion to the design steady state in the presence of disturbances, suppressing intolerable overshoots, or meeting certain optimality criteria [18, 48, 78]. Traditionally, the selection of the nonlinear regulator parameters p has been achieved through heuristics or trial-and-error type of approaches [48, 78]. In

the context of the present study however, p would be optimally selected through the optimization of a physically meaningful performance index and the ideas presented in the previous section.

The controlled (regulated) reactor dynamics can be easily obtained by inserting (1.28) into the reactor dynamics equation (1.27):

$$x(k+1) = \varphi\left(x(k), \kappa\left(x(k); p\right)\right) \tag{1.29}$$

Let:

$$\begin{aligned} J(p) &= \sum_{k=0}^{\infty} \left\{||x(k)||^2 + \rho||u(k)||^2\right\} \\ &= \sum_{k=0}^{\infty} \left\{||x(k)||^2 + \rho||\kappa\left(x(k), p\right)||^2\right\} \end{aligned} \tag{1.30}$$

The choice of the above quadratic performance index is physically meaningful and can be justified by the fact that it contains a term: $||x(k)||^2$ that captures the distance of the current dynamic reactor state from the reference equilibrium point (assumed to be the origin) as the regulator forces the reactor to asymptotically reach it, and a second one: $||u(k)||^2$ that represents a measure of the necessary control effort in order to successfully perform the system's regulation at the origin. Please notice, that since the regulation law introduces the parameters p, the performance index J will depend on p as well.

To simplify the notation, let us define the vector function $\Phi((x(k); p) = \varphi(x(k), \kappa(x(k); p))$ and the positive definite scalar function $Q(x(k); p) = \|x(k)\|^2 + \rho\|\kappa(x(k); p)\|^2$. Under the above notation, the controlled reactor dynamics (1.29) and the performance index $J(p)$ can be rewritten as follows:

$$x(k+1) = \Phi(x(k); p) \tag{1.31}$$

$$J(p) = \sum_{k=0}^{\infty} Q(x(k); p) \tag{1.32}$$

Please notice, that the problem under consideration is now formulated exactly as the one presented in the previous section. However, the dependence of both the

controlled system dynamics and the performance index on the controller parameter vector p is now explicit.

As intuitively expected, the regulator (1.28) has rendered the controlled reactor dynamics stable, and therefore, the Zubov-like functional equation:

$$V(\Phi(x(k);p)) - V(x(k)) = -Q(x;p) \tag{1.33}$$

admits a unique locally analytic solution $x(0)$,which is a Lyapunov function that explicitly depends on the controller parameters p^*. Moreover, the performance index $J(p)$ is exactly the value of V at the initial state:

$$J(p) = V((x(0);p) \tag{1.34}$$

Therefore, given an initial condition $x(0)$, the optimal values for the controller parameters p^* can be obtained through the solution of the following finite-dimensional parametric optimization problem:

$$p^* = \arg\min_{p\in P} J(p) = \arg\min_{p\in P} V(x(0);p) \tag{1.35}$$

subject to a set of constraints that guarantee that the Jacobian matrix $\dfrac{\partial\Phi}{\partial x}(0;p)$ has stable eigenvalues (stability requirement). The above static optimization problem is a nonlinear mathematical program for which a multitude of numerically efficient algorithms and techniques exist in the literature [31]. Furthermore, the set of admissible parameters P and the constraints associated with the reactor stability assumptions render this optimization problem a constrained one. It should be pointed out, that the proposed approach can be computationally demanding under certain circumstances for higher-order large-scale systems due to the formulation of the optimization problem that presupposes the symbolic calculation of the solution of the functional equation (1.11). However, the comparative advantage of the proposed method is that it allows a more transparent and insightful analysis of the reactor dynamics to be performed, establishing a very important system-theoretic link between stability and a

physical measure of performance such as an optimality criterion [51, 75, 80]. Furthermore, as it will be seen in the next section's illustrative example, the availability of enhanced computational capabilities naturally generates new interest in the practical application of the above ideas and the proposed optimization scheme.

1.4 Illustrative example

To illustrate the main aspects and different steps of the proposed algorithmic approach, let us consider the series/parallel Van de Vusse reaction [100] taking place in a continuous stirred tank chemical reactor in isothermal operation [18, 86]:

$$\begin{gathered} A \rightarrow B \rightarrow C \\ 2A \rightarrow D \end{gathered} \tag{1.36}$$

with rates of formation of species A and B given by:

$$r_A = -k_1 C_A - k_3 C_A^2 \tag{1.37}$$

$$r_B = k_1 C_A - k_2 C_B^2 \tag{1.38}$$

Under the assumption that the feed stream consists of pure A, the mass balance equations for species A and B lead to the following nonlinear dynamic process model [100]:

$$\begin{aligned} \frac{dC_A}{dt} &= f_1\left(C_A, C_B, \frac{F}{V}\right) = \frac{F}{V}(C_{A_0} - C_A) - k_1 C_A - k_3 C_A^2 \\ \frac{dC_B}{dt} &= f_2\left(C_A, C_B, \frac{F}{V}\right) = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B \end{aligned} \tag{1.39}$$

where is the inlet flow rate of A, V is the volume of the reactor that is considered to be constant during the operation, C_A and C_B are the concentrations of species A and B in the reactor respectively, and C_{A_0} is the concentration of A in the feed stream. The control objective is to regulate the concentration C_B at a constant desired level (set-point) by manipulating the dilution rate (F/V).

The above reactor-dynamic model is mathematically represented in the continuous time domain. In order to digitally control and optimize the reactor dynamic behavior a discretization method is needed [18, 28, 78].

Any type of time-discretization can be used in principle, but for the sake of simplicity let us employ a basic Euler's discretization scheme for the nonlinear ODEs (1.39). One obtains:

$$\begin{aligned} C_A(k+1) &= C_A(k) + \delta f_1\left(C_A(k), C_B(k), (F/V)(k)\right) \\ &= \varphi_1\left(C_A(k), C_B(k), (F/V)(k)\right) \\ C_B(k+1) &= C_B(k) + \delta f_2\left(C_A(k), C_B(k), (F/V)(k)\right) \\ &= \varphi_2\left(C_A(k), C_B(k), (F/V)(k)\right) \end{aligned} \tag{1.40}$$

where k is the discrete-time index, and δ is the discretization time-step. Please notice that the time step has been chosen small enough compared to the dominant process time constant in order to avoid numerical instability. Under the above assumption, it was numerically verified that the nonlinear difference equations (1.40) capture quite adequately the reactor's actual dynamic behavior. Let us now consider the problem of optimally calculating the digital controller parameters for a specific step change in the set point. In all ensuing simulation runs the set-point for C_B was chosen to be $C_{B,S} = 1.05 gmol/l$ with the corresponding reactor equilibrium state being at:

$$\begin{aligned} (F/V)_S &= 28.428 l/h \\ C_{A_S} &= 2.697 gmol/l \\ C_{B_S} &= 1.05 gmol/l \end{aligned}$$

In order to conform to the theory presented in previous sections and facilitate the pertinent calculations, deviation variables with respect to the above reference steady state are defined as follows:

$$\begin{aligned} x_1(k) &= C_A(k) - C_{A_S} \\ x_2(k) &= C_B(k) - C_{B_S} \\ u(k) &= (F/V)(k) - (F/V)_S \end{aligned} \tag{1.41}$$

Notice, that the origin becomes now the reference equilibrium point when deviation variables are used.

Using the above set of deviation variables the reactor dynamic model can be put in the following form:

$$\begin{aligned} x_1(k+1) &= \bar{\varphi_1}\left(x_1(k), x_2(k), u(k)\right) \\ x_2(k+1) &= \bar{\varphi_2}\left(x_1(k), x_2(k), u(k)\right) \end{aligned} \tag{1.42}$$

with:

$$\begin{aligned} \bar{\varphi_1}\left(x_1(k), x_2(k), u(k)\right) &= \varphi_1\left(x_1(k) + C_{A_S}, x_2(k) + C_{B_S}, u(k) + (F/V)\right) \\ \bar{\varphi_2}\left(x_1(k), x_2(k), u(k)\right) &= \varphi_2\left(x_1(k) + C_{A_S}, x_2(k) + C_{B_S}, u(k) + (F/V)\right) \end{aligned}$$

Parameter	Value
k_1	$10h^{-1}$
k_2	$100h^{-1}$
k_3	$10l/gmol \cdot h$
C_{A_0}	$10gmol/h$

Table 1: Process Parameter Values

The numerical values used for the various process parameters are tabulated in Table 1.

A simple digital linear regulation law was applied to the system:

$$u(k) = -p_1 x_1(k) - p_2 x_2(k) \tag{1.43}$$

where $\{p_1, p_2\}$ are the regulator parameters to be optimized [78]. According to the proposed method, their optimal values can be obtained by minimizing the following performance index:

$$\begin{aligned} J(p_1, p_2) &= \sum_{k=0}^{\infty} \left[x_2(k)\right]^2 + \rho\left[u(k)\right]^2 \\ &= \sum_{k=0}^{\infty} \left[x_2(k)\right]^2 + \rho\left[-p_1 x_1(k) - p_2 x_2(k)\right]^2 \end{aligned} \tag{1.44}$$

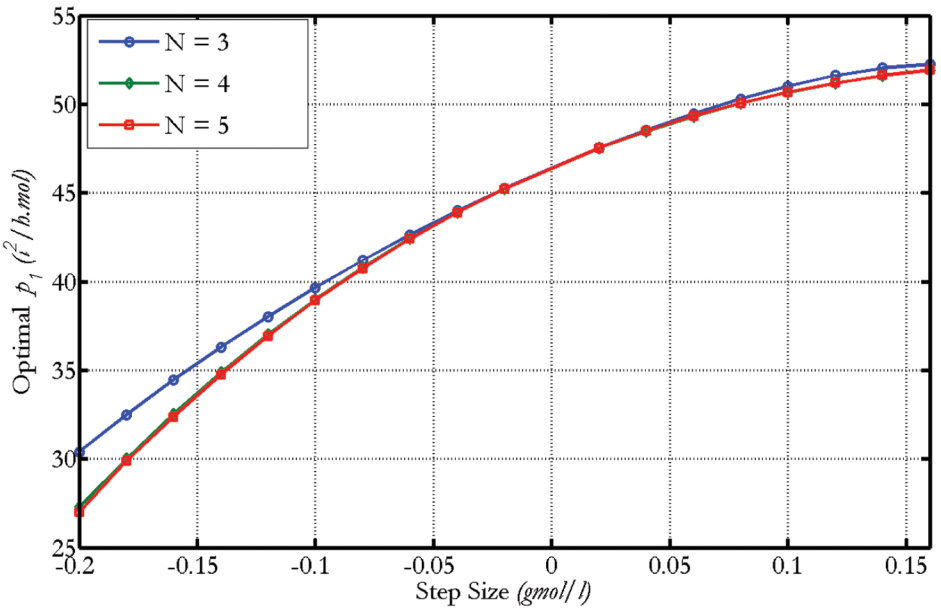

Figure 1.1: Optimal values of p_1 as a function of the size of the step change in the set point

Applying the method described in Sections 2 and 3, the above performance index can be explicitly calculated as follows:

$$J(p_1, p_2) = V\left(x_1(0), x_2(0); p_1, p_2\right) \tag{1.45}$$

where $V(x_1, x_2; p_1, p_2)$ is the solution of the following Zubov-like functional equation:

$$\begin{aligned} V\left(\bar{\varphi}_1(x_1, x_2, -p_1x_1 - p_2x_2), \bar{\varphi}_2(x_1, x_2, -p_1x_1 - p_2x_2)\right) - V(x_1, x_2) \\ = -x_2^2 - \rho(p_1x_1 + p_1x_2)^2 \end{aligned} \tag{1.46}$$

The above functional equation was solved symbolically using the software package MAPLE and the series solution method for a finite truncation order N. The result was evaluated at the chosen initial condition and the function $V^N\left(x_1(0), x_2(0); p_1, p_2\right)$ was minimized using the nonlinear programming library of MAPLE (see Appendix A):

$$p^* = \arg\min_{p \in P} J(p_1, p_2) = \arg\min_{p \in P} V\left(x_1(0), x_2(0); p_1, p_2\right) \tag{1.47}$$

The optimal values of p_1 and p_2 for different values of the step size and different orders of truncation N are presented in Figures 1.1 and 1.2. These values were

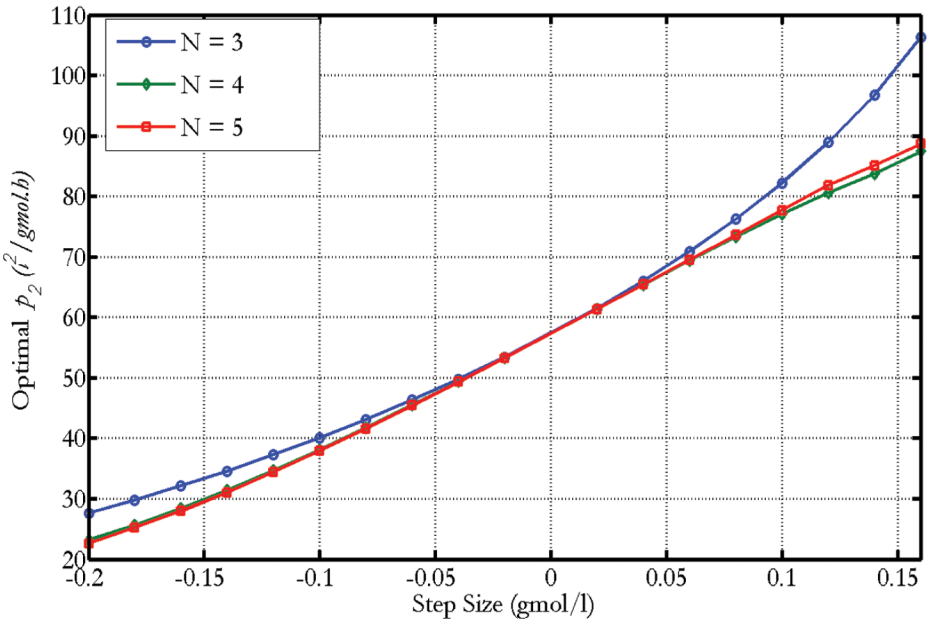

Figure 1.2: Optimal values of p_2 as a function of the size of the step change in the set point

obtained with a weight coefficient $\rho = 10^{-5}$. Please notice that the step size is a measure of how drastic the disturbance effect has been, driving the system far from the desired final equilibrium state.

As suggested by Figures 1.1 and 1.2, the optimal values of the regulator parameters p_1 and p_2 are highly dependent on the step size. This is of course intuitively expected due to the nonlinear nature of the system under study. An additional piece of information provided by these figures, is that fast convergence is attained, as the order of series truncation N increases. In this particular case study, an order of truncation $N = 4$ is enough for a satisfactory approximation.

Figures 1.3 and 1.4 show the optimal responses obtained with different values of the weight coefficient ρ. As expected, when the weight coefficient ρ attains small values the system's response is very fast, but at the expense of unrealistic values of the dilution rate. Indeed, as we lower the value of ρ, we tend not to drastically penalize the control effort needed for reactor regulation, the regulator becomes more

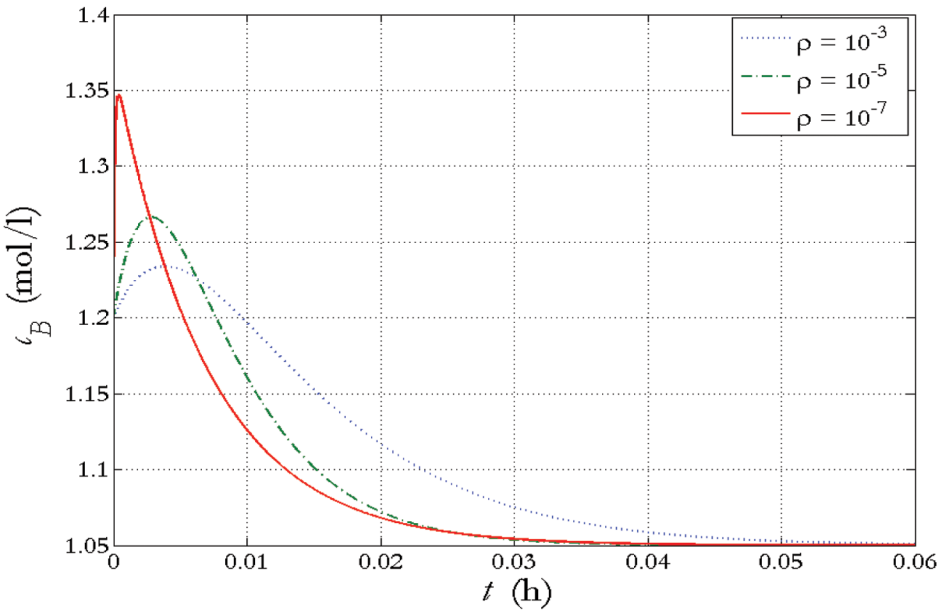

Figure 1.3: Optimal output responses to a step change in the set point from $1.2 gmol/l$ to $1.05 gmol/l$ with different weight coefficient

aggressive, the reactor response that it induces faster, but the values of the input variable that are generated may become physically unrealizable. The opposite effect is naturally observed for larger values of the weight coefficient ρ. In this case, a large control effort u is severely penalized, the regulator becomes less aggressive enforcing a dynamically more sluggish response and reversion to the desired reference equilibrium state.

Finally, Figures 1.5 and 1.6 illustrate how the method described in Section 2 is used to obtain stability region estimates. This is a very useful feature of the proposed method, because it also equips us with the capacity to assess the reactor's stability characteristics under the optimal regulator parameters. In particular, stability region estimates were obtained by considering the largest contour curve of the function $V(x)$ which is tangent to the $\Delta V^{(N)}(x) = 0$ curve, and wholly contained in the region where $\Delta V^{(N)}(x) < 0$ [75, 80].

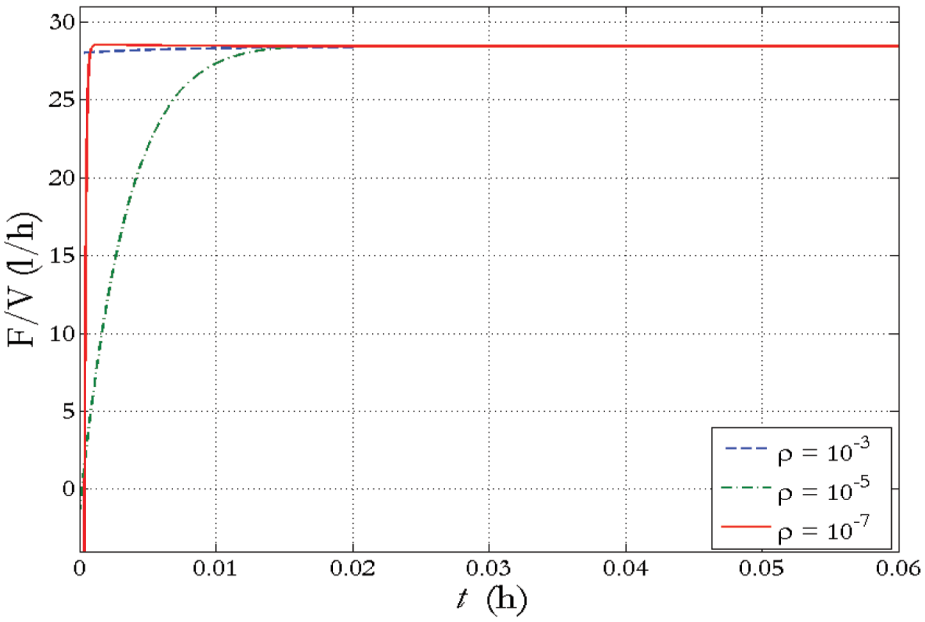

Figure 1.4: Optimal intput responses to a step change in the set point from $1.2 gmol/l$ to $1.05 gmol/l$ with different weight coefficient

1.5 Concluding Remarks

A systematic methodology was presented that responds to the need of optimizing the digitally controlled reactor dynamics. The method is based on the explicit calculation of the value of a physically meaningful performance index through the solution of a Zubov-like functional equation. A static optimization scheme provides the optimal reactor regulator parameters through the minimization of the parameterized performance index. The properties of the solution of the Zubov-like functional equation allow the derivation of stability region estimates associated with the controlled reactor dynamics. Finally, the proposed method was illustrated in a nonlinear chemical reactor example and its satisfactory performance demonstrated via simulation studies.

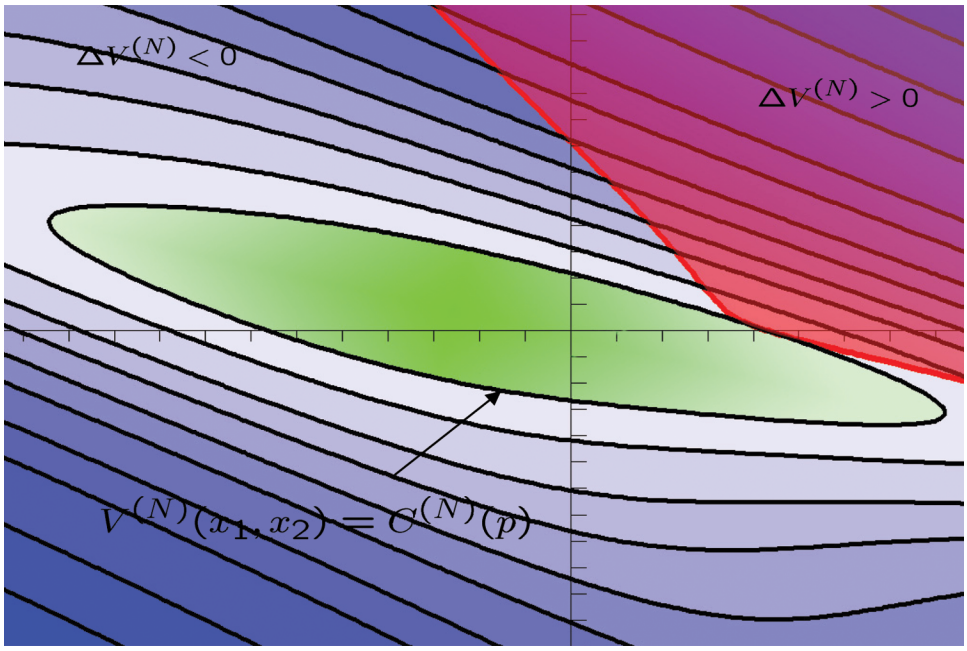

Figure 1.5: Geometric interpretation of the method for estimating the stability region with $N = 4$, $p_1 = 46.4l^2/h \cdot mol$, $p_2 = 57.3l^2/h \cdot mol$

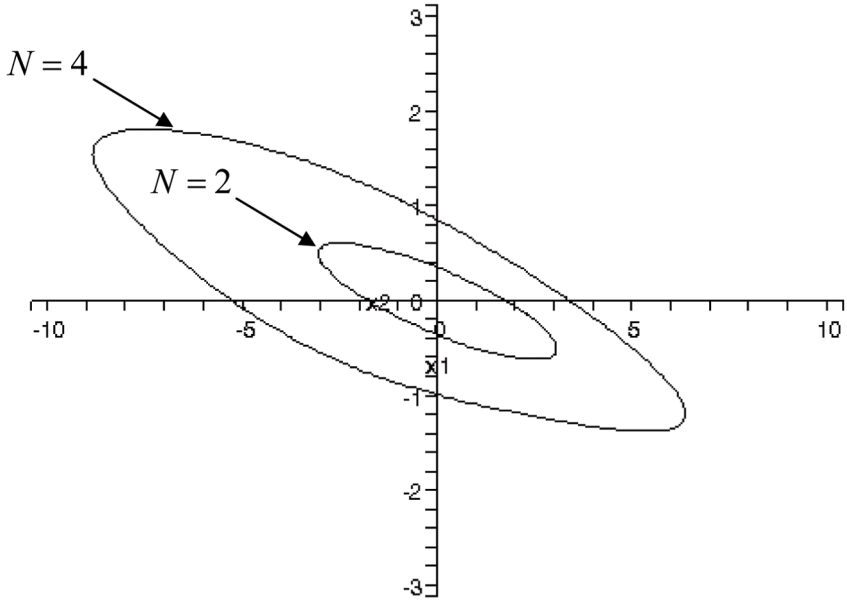

Figure 1.6: Stability region estimates for $N = 2$ and $N = 4$ with $p_1 = 46.4l^2/h \cdot mol$, $p_2 = 57.3l^2/h \cdot mol$

CHAPTER 2

A Model-Based Characterization of the Long Term Asymptotic Behavior of Nonlinear Discrete-Time Processes

2.1 Introduction

The chemical engineering literature is dominated by physical and (bio)chemical processes that exhibit nonlinear behavior and are typically modeled by systems of nonlinear ordinary (ODEs) or partial differential equations (PDE) in the continuous-time domain , or systems of nonlinear difference equations (DEs) in the discrete-time domain [8,18,79,82]. Furthermore, accompanying the growing computational capacities, efficient and accurate discrete-time dynamic process modeling techniques have been developed, allowing the digital simulation, analysis and characterization of complex process dynamic behavior to be performed in a thorough manner. Particularly, the development of efficient discretization techniques, applied to a system of ODEs/PDEs or various process identification methods in the continuous-time domain, can provide us with discrete-time dynamic models characterized by a high degree of fidelity, allowing insightful theoretical and computational investigations on the process dynamic

behavior. Nevertheless, despite the fact that the dynamic analysis of linear processes can be performed with rigor [8,27,82], the task remains very challenging for nonlinear processes. Particular efforts in nonlinear dynamic analysis have been concentrated on reducing the dimensionality of the original problem [3, 11, 21, 33, 34, 45, 54, 77, 84, 99]. Within the above framework, the restriction of the system dynamics on an invariant manifold results in a reduced-order dynamic model, and essentially determines the long-term asymptotic behavior, since the original transition or approach to the manifold can be proven to be rather fast under certain conditions. Some representative recent applications of invariant manifold theory to chemical reaction systems for model-reduction purposes can be found in various publications [6,43,70,72,83,97,101]. Furthermore, the study of invariant manifolds has been historically conducted in connection with the existence problem of a stable, unstable or center manifold, stability, as well as bifurcation analysis [99]. One should however notice that the stable and center manifold theory presupposes the successful transformation of the original nonlinear dynamical system into one whose Jacobian matrix of the linearized system around the equilibrium point of interest is in Jordan canonical form, and the corresponding stable, unstable and center eigenmodes appear as decoupled (the state space of interest being the direct sum of the stable, unstable and center eigenspaces) [99]. The later requirement, while always achievable through a coordinate transformation, may result in a computationally demanding numerical problem particularly for higher order systems, such as the ones obtained from discretization or modal decomposition techniques applied to distributed parameter systems [18]. Following the ideas used for the standard stable and center manifold theory, conceptual and technical extensions have been developed in the case of singularly perturbed systems, where the classification of the corresponding invariant manifolds as slow and fast is a natural consequence of the two-time scale separation property [30,64]. Moreover, a conceptually similar geometric notion of a positively invariant finite-dimensional manifold was

introduced in the study of the dynamic model reduction problem for parabolic PDE systems under the name of inertial manifold [18]. One should notice that unlike the existence theorems available for the standard stable and center manifold theory [99], inertial manifolds were proven to exist only for certain classes of parabolic PDEs (on a case-by-case basis). However, there are systematic techniques available for computing, up to a certain degree of accuracy, approximations of the so-called manifold equation [18]. Finally, research results on symmetry-induced generalized invariants for distributed parameter systems were also reported in [81].

A systematic approach is proposed in the present research study [58], to rigorously address the problem of quantitatively characterizing the long-term dynamic behavior of non-linear discrete-time processes using the notion of invariant manifold. The problem under consideration is naturally formulated as a system of nonlinear functional equations (NFEs), and a set of rather general solvability conditions can be derived. This set of conditions guarantees the existence and uniqueness of a locally analytic solution, which is then proven to represent a locally analytic invariant manifold of the nonlinear discrete-time process dynamincs considered. However, within the proposed framework of analysis, the formulation of the problem of interest does not require the special structure of the Jacobian eigenspace of the linearized system associated with the classical stable and center manifold theory, thus effectively overcoming the associated problems of computing the requisite transformation into the Jordan canonical form with the explicit decoupling of the stable, unstable and center eigenspaces, as well as the numerical solution to the associated eigenstructure problem [99]. Furthermore, the local analyticity property of the invariant manifold map enables the development of a series solution method, which can be easily implemented using MAPLE. Under a certain set of conditions, it can be shown that the invariant manifold computed attracts all system trajectories, and therefore, the asymptotic process response and long-term dynamic behavior are calculated through

the restriction of the discrete-time process dynamics on the invariant manifold.

The present chapter is organized as follows: Section 2.2 contains some mathematical preliminaries that are necessary for the ensuing theoretical developments. The chapter's main results are presented in Section 2.3, accompanied by remarks and comments on their potential use for process performance monitoring purposes. An illustrative case study of an enzymatic bioreactor is presented in Section 2.4, followed by a few concluding remarks in Section 2.5.

2.2 Mathematical preliminaries

A nonlinear discrete-time dynamic process model is considered with a state space representation of the following form:

$$x(k+1) = F\left(x(k), w(k)\right) \tag{2.1}$$

which is driven by the states of an exogenous nonlinear discrete-time autonomous dynamical system:

$$w(k+1) = G\left(w(k)\right) \tag{2.2}$$

where $k \in \mathbb{N}$ is the discrete-time index and $\mathbb{N}$ the set of positive integers, $x \in U^n \subset \mathbb{R}^n$ is the process state vector, $w \in U^m \subset \mathbb{R}^m$ is the state vector associated with dynamics (2.2), and U^n, U^m are open subsets of the Euclidean spaces R^n and R^m respectively. Notice that the above dynamic process description in the discrete-time domain may represent a process whose dynamics (2.1) is driven by:

(i) the input/disturbance dynamics (2.2), where input or disturbance changes are modeled and generated as outputs of the exogenous dynamical system (2.2), or

(ii) a time-varying process parameter vector $w(k)$ that follows dynamics (2.2) and models phenomena such as catalyst deactivation, enzymatic thermal deactivation, heat-transfer coefficient changes, time-varying (bio)chemical kinetic parameters, etc., or

(iii) the autonomous dynamics of an upstream process modeled by (2.2), in which case, a cascade connection of the two nonlinear processes results in the "block-triangular" structure (2.1)-(2.2).

As stated in the introductory Section 2.1 ,it is also assumed that the discrete-time dynamic process model (2.1)-(2.2) is obtained:

(a) either through the deployment of efficient and accurate discretization methods for the original continuous time process (modeled by a system of nonlinear ordinary (ODEs) or partial differential equations (PDEs) that mathematically reflect the underlying fundamental phenomena) or

(b) through direct identification methods.

It is also assumed that the $F(x, w)$ and $G(w)$ maps of the discrete-time dynamics (2.1)-(2.2) are real-analytic vectors functions defined on $U^n \times U^m$ and U^m respectively. Without loss of generality, let the origin $x^0 = 0$ be an equilibrium point of (2.1): $F(0, 0) = 0$, that corresponds to $w^0 = 0$ with $G(0) = 0$. The following assumption is also made:

Assumption 2.1.

Matrix A:

$$A = \frac{\partial G}{\partial w}(0) \tag{2.3}$$

has non-zero eigenvalues $k_i, (i = 1, ..., m)$ that all lie inside or outside the unit disk (Poincaré domain [3]). This assumption implies that the w-dynamics is either locally asymptotically stable or unstable, and that the $G(w)$ map is locally invertible around $w^0 = 0$.

The original nonlinear discrete-time dynamic process model (2.1)-(2.2) may therefore be rewritten as follows:

$$\begin{aligned} x(k+1) &= Bx(k) + Cw(k) + f\left(x(k), w(k)\right) \\ w(k+1) &= Aw(k) + g\left(w(k)\right) \end{aligned} \tag{2.4}$$

where B,C are constant matrices with appropriate dimensions, and $f(x,w)$, $g(w)$ are real analytic functions of x and w with $f(0,0) = g(0)$, and $\dfrac{\partial f}{\partial x}(0,0) = \dfrac{\partial f}{\partial w}(0,0) = \dfrac{\partial g}{\partial w}(0) = 0$.

The following definitions are essential for the ensuing developments.

Definition 2.1.

A set $S \in \mathbb{R}^{m+n}$ is said to be *invariant* under the flow of the nonlinear discrete-time dynamics 2.4 if for each $(x_0, w_0) \in S$, the orbit $\Omega = \{(x(k), w(k)), k \in \mathbb{N}\}$ satisfying $((x(k=0), w(k=0)) = (x_0, w_0)$, is such that $(x(k), w(k)) \in S$ for all $k \in \mathbb{N}$ [99].

Definition 2.2.

An invariant set $S \subset \mathbb{R}^{m+n}$ passing through the origin $(x^0, w^0) = (0,0)$ is said to be *an locally analytic invariant manifold* of (2.4) , if S has the local topological structure of an analytic manifold around the origin [99].

2.3 Main results

Together with the original nonlinear discrete-time input-driven dynamic process model (2.4) an associated system of nonlinear first-order functional equation (NFEs) is also considered:

$$\begin{aligned} \pi(Aw + gw) &= B\pi(w) + Cw + f(\pi(w), w) \\ \pi(0) &= 0 \end{aligned} \tag{2.5}$$

where $\pi\colon \mathbb{R}^m \to \mathbb{R}^n$ is the unknown vector function of 2.5.

The following technical lemma reported in [55] is necessary.

Lemma 2.1.

Suppose that for the nonlinear discrete-time dynamic process model (2.1)-(2.2) Assumption 2.1 holds true.

Consider the system of NFEs (2.5) and assume the eigenvalues $k_i, (i = 1, ..., m)$ *of matrix* $A = \dfrac{\partial G}{\partial w}(0)$ *are not related to the eigenvalues* $\lambda_i, (i = 1, ..., n)$ *of matrix* $B = \dfrac{\partial F}{\partial x}(0, 0)$ *through any equation of the following type:*

$$\prod_{i=1}^{m} k_i^{d_i} = \lambda_j \tag{2.6}$$

$(j = 1, ..., n)$*, where all the* d_i*'s are nonnegative integers satisfying the condition:*

$$\sum_{i=1}^{m} d_i > 0 \tag{2.7}$$

Then, the associated system of NFEs (2.5) admits a unique locally analytic solution $\pi(w)$ *in a neighborhood of* $w = 0$

Remark 2.1. Let us now consider the linear case where $G(w) = Aw$ and $F(x, w) = Bx + Cw$, with A, B, C being constant matrices with appropriate dimensions. The unique solution to the system of functional equations (2.5) is given by: $\pi = \Pi w$ where Π is the solution of the Lyapunov-Sylvester matrix equation:

$$\Pi A - B\Pi = C \tag{2.8}$$

It is known that the above linear matrix equation (2.8) admits a unique solution Π as long as the eigenspectra of matrices A, B are disjoint [38]. Notice, that the latter is guaranteed by the assumptions of Lemma 2.1, and, therefore, the linear result can be naturally reproduced.

We are now in a position to present this chapter's main results.

Theorem 2.1.

Suppose that for the nonlinear discrete-time dynamic process model (2.1)-(2.2) Assumption 2.1 holds true, as well as the assumptions of Lemma 2.1.

Then, there exists a neighborhood $V \subset \mathbb{R}^m$ *of* $w^0 = 0$*, and a unique locally analytic mapping* $\pi \colon V \to \mathbb{R}^n$ *such that:*

$$S = \{(x, w \in \mathbb{R}^n \times V \colon x = \pi(w), \pi(0) = 0\} \tag{2.9}$$

is an analytic local invariant manifold of (2.1)-(2.2) (in the sense of Definition 2.2) that passes through the origin $(x^0, w^0) = (0, 0)$*, where* $\pi(w)$ *is the unique solution of the associated system of NFEs (2.5).*

Proof of Theorem 2.1. For the graph of the mapping $x = \pi(w)$ to be a local invariant manifold that passes through the origin $(x^0, w^0) = (0, 0)$, it has to satisfy the following system of invariance NFEs:

$$\begin{gathered} \pi(Aw + g(w)) = B\pi(w) + Cw + f(\pi(w), w) \\ x(0) = 0 \end{gathered} \tag{2.10}$$

The above equation can be easily deduced by applying the one-step forward in time-operator on $x = \pi(w)$ and along an arbitrary solution curve $(x(k), w(k))$ of (2.1) and (2.2) which belongs to the manifold of interest, i.e. identically satisfies: $x(k) = \pi(w(k))$.

The above system of invariance NFEs (2.10) is exactly the system of NFEs (2.5) associated with the original discrete-time dynamics and the maps $F(x, w)$ and $G(w)$. Under the assumptions stated, the above system of NFEs (2.10) admits a unique and locally analytic solution in a neighborhood $V \subset \mathbb{R}^m$ of $w^0 = 0$ due to Lemma 2.1. Therefore:

$$S = \{(x, w \in \mathbb{R}^n \times V \colon x = \pi(w), \pi(0) = 0\} \tag{2.11}$$

is indeed an analytic local invariant manifold of (2.1) and (2.2). □

Remark 2.2. The invariant manifold $x = \pi(w)$ of Theorem 2.1, that is computed through the solution of the associated system of NFEs (2.5), may coincide with the

system's stable or unstable manifold under certain conditions. For a more thorough discussion on this matter, the interested reader is refered to [55].

Remark 2.3. For practical reasons, one must provide a solution scheme for the system of invariance NFEs (2.5).

Notice that $F(x,w), G(w)$ and $\pi(w)$ are locally analytic, and therefore, the proposed method suggests their expansion in Taylor series, followed by a procedure that equates the same order Taylor coefficients of both sides of (2.5). This procedure leads to recursion formulas, through which one can calculate the Nth-order Taylor coefficients of the unknown solution $x = \pi(w)$, given the Taylor coefficients of $x = \pi(w)$ up to order $N-1$ by solving a system of linear equations. In the derivation of the recursion formulas, it is convenient to use the following tensorial notation:

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 refers to the corresponding column of the matrix.

b. The partial derivatives of the μ-th component $F_\mu(x,w)$ of the vector function $F(x,w)$ evaluated at $(x,w) = (x_0, w_0)$ are denoted as follows:

$$\begin{aligned} F_\mu^i &= \frac{\partial F_\mu}{\partial x_i}(0,0) \\ F_\mu^{ij} &= \frac{\partial^2 F_\mu}{\partial x_i \partial x_j}(0,0) \\ F_\mu^{ijk} &= \frac{\partial^3 F_\mu}{\partial x_i \partial x_j \partial x_k}(0,0), etc... \end{aligned}$$

where i, j, k=1, ..., n.

c. The partial derivatives of the μ-th component $F_\mu(x,w)$ of the vector function $F(x,w)$ with respect to the variables w evaluated at $(x,w) = (0,0)$ are denoted as follows: $\bar{F}_\mu^i = \dfrac{\partial^i F_\mu}{\partial w^i}(0,0)$, etc.

d. The standard summation convention where repeated upper and lower tensorial indices are summed up.

Under the above notation, the l-th component $pi_l(w)$ of the unknown solution $\pi(w)$ can be expanded in a multivariate Taylor series as follows:

$$\begin{aligned}\pi_l(w) = \frac{1}{1!}\pi_l^{i_1} w_{i_1} + \frac{1}{2!}\pi_l^{i_1 i_2} w_{i_1} w_{i_2} + ... \\ + \frac{1}{N!}\pi_l^{i_1 i_2 ... i_N} w_{i_1} w_{i_2} ... w_{i_N} + ...\end{aligned} \tag{2.12}$$

and similarly for $F(x,w)$ and $G(w)$. Inserting the Taylor expansions of $\pi(w)$,$F(x,w)$ and $G(w)$ into (2.5) and matching the Taylor coefficients of the same order, the following relation for the Nth order can be obtained:

$$\begin{aligned}\sum_{L=1}^{N} \sum_{0 \le m_1 \le ... \le m_L} \pi_l^{j_1 ... j_L} G_{j_1}^{m_1} ... G_{j_L}^{m_L} \\ = F_l^{\mu} \pi_{\mu}^{i_1 ... i_N} + \bar{F}_l^{i_1 ... i_N} + f_l^{i_1 ... i_N}(\pi^{i_1 ... i_{N-1}})\end{aligned} \tag{2.13}$$

where $i_1, ..., i_N = 1, ..., m, l = 1, ..., n, \sum_{j=1}^{L} m_j = N$ and $f_l^{i_1 ... i_N}(\pi^{i_1 ... i_{N-1}})$ is a function of Taylor coefficients of the unknown solution $\pi(w)$ calculated in the previous recursive steps. Note that the second summation symbol in (2.13) suggests summing up the relevant quantities over the $\frac{N!}{m_1! ... m_L!}$ possible combinations to assign the N indices $(i_1, ...i_N)$ as upper indices to the L positions $G_{j_1} ... G_{j_L}$, with m_1 of them being put in the first position, m_2 of them in the second position, etc. $(\sum_{j=1}^{L} m_j = N)$. Furthermore, notice that equations (2.13) represent a set of linear algebraic equations in the unknown coefficients $\pi_{\mu}^{i_1, ... i_N}$. Finally, a MAPLE code similar to the code found in Appendix A has been developed to automatically compute the Taylor coefficients of the unknown solution $x = \pi(w)$ of NFEs (2.5).

Theorem 2.2. *Let matrix B have stable eigenvalues ($|\lambda_i| < 1, i = 1, ...n$) and all assumptions of Theorem 2.1 hold true. Furthermore, let S defined in equation (2.9) be an invariant manifold of (2.1)-(2.2), where $\pi(w)$ is the solution to the associated system of invariance NFEs (2.5) and $(x(k), w(k))$ a solution curve of (2.1)-(2.2).*

There exists a neighborhood U^0 of the origin $(x^0, w^0) = (0, 0)$ and a real number $M \in (0, 1)$ such that, if $(x(0), w(0) \in U^0)$, then:

$$||x(k) - \pi((w(k))||_2 \leq (M)^k ||x(0) - \pi(w(0))||_2 \tag{2.14}$$

Proof of Theorem 2.2. Denote by z the "off-manifold" coordinate:

$$z(k) = x(k) - \pi(w(k)) \tag{2.15}$$

whose dynamics is described by:

$$\begin{aligned} z(k+1) &= B(z(k) + \pi(w(k))) + Cw(k) + f(z(k) + \pi(w(k)), w(k)) \\ &\quad -B\pi(w(k)) - Cw(k) - f(\pi(w(k)), w(k)) \\ &= Bz(k) + N(z(k), w(k)) \end{aligned} \tag{2.16}$$

where: $N(z, w) = f(z + \pi(w), w) - f(\pi(w), w)$. Notice that $N(z, w)$ is a real analytic vector function with: $N(0, 0) = 0$ and no linear terms in z: $\frac{\partial N}{\partial z}(0, 0) = 0$. Consequently: $\frac{||N(z,w)||_2}{||z||_2} \to 0$ as $||z||_2 \to 0$, and thus, for an arbitrary constant $L > 0$ there exist positive ρ_1, ρ_2, such that in the domain: $\|z\|_2 < \rho_1, \|w\|_2 < \rho_2$ the following inequality holds:

$$\|N(z, w)\|_2 < L\|z\|_2 \tag{2.17}$$

Furthermore, since matrix B has all its eigenvalues with modulus less than one, there exist positive constants $\beta \in (0, 1)$ and γ such that [11, 27]:

$$\|(B)^k y\|_2 \leq \gamma(\beta)^k \|y\|_2 \tag{2.18}$$

for all $y \in \mathbb{R}^n$.

From equation (2.16), one obtains [27]:

$$z(k) = (B)^k z(0) + \sum_{j=0}^{k-1} (B)^{k-j-1} N(z(j), w(j)) \tag{2.19}$$

and therefore:

$$\|z(k)\|_2 \leq \gamma(\beta)^k \|z(0)\|_2 + \sum_{j=0}^{k-1} \gamma L(\beta)^{k-j-1} \|z(j)\|_2 \tag{2.20}$$

or:

$$(\beta)^{-k}\|z(k)\|_2 \leq \gamma \left\{ (\|z(0)\|_2 + \sum_{j=0}^{k-1} L(\beta)^{-j-1}\|z(j)\|_2 \right\} \tag{2.21}$$

Applying Gronwall-Bellman's inequality [27], it can be deduced that:

$$\begin{aligned} (\beta)^{-k}\|z(k)\|_2 &\leq \|z(0)\|_2 \prod_{j=0}^{k-1}(1+\gamma L(\beta)^{-1}) \\ \Rightarrow (\beta)^{-k}\|z(k)\|_2 &\leq \|z(0)\|_2(\beta)^{-k}(\beta+L\gamma)^k \\ \Rightarrow \|z(k)\|_2 &\leq (M)^k\|z(0)\|_2 \\ \Rightarrow \|x(k)-\pi(w(k))\|_2 &\leq (M)^k\|x(0)-\pi((w(0))\|_2 \end{aligned} \tag{2.22}$$

where $M = \beta + L\gamma$. Since L can be made arbitrarily small, let is choose $L < \frac{1-\beta}{\gamma}$ so that $0 < M < 1$, and the proof is complete. □

Theorem 2.2 states that, as time tends to infinity (asymptotically), any trajectory of the overall system (2.1)-(2.2) starting at a point sufficiently close to the origin converges to a trajectory that lies entirely on the invariant manifold S. Therefore, the long-term asymptotic response of the nonlinear process (2.1) in the presence of the w-dynamics (2.2) is given by:

$$x(k) \underset{k\to\infty}{\approx} \pi(w(k)) \tag{2.23}$$

where $\pi(k)$ is the solution of the associated system of invariance NFEs (2.5). Equivalently, under the assumption of Theorem 2.2, the invariant manifold S (2.9) computed through the associated system of NFEs (2.5) is rendered locally "attractive" [11], and the restriction of the process dynamics on the aforementioned manifold (often termed as the "slow dynamics" or the "dynamics on the slow manifold") embedded in state space determines the long-term asymptotic behavior of the process [99]:

$$\begin{aligned} w(k+1) &= G(w(k)) \\ x(k) &\underset{k\to\infty}{\approx} \pi(w(k)) \end{aligned} \tag{2.24}$$

Remark 2.4. The seminal work presented in [37, 93, 98] on chemical reaction invariants/variants is fundamentally different in scope and technically from the proposed one. In their respective framework of analysis, the above publications aim at identifying classes of linear variable transformations that reflect the basic underlying conservation laws (for atoms, charge and energy) dictated by stoichiometry, kinetics, thermodynamics and possibly reactor operating conditions (linear invariant subspaces). Therefore, the above approaches identify all constraints that the process dynamics ought to obey and typically lead to the smallest number of independent transformed variables whose dynamic evolution suffices for a unique characterization of the process dynamic state. The proposed work presupposes that the state space representation (2.1) and (2.2) is already realized by the smallest number of independent state variables (for simple systems, this task can be easily carried out; the aforementioned approaches focus primarily on complex chemical reaction systems with numerous reactions and species for which the task is not trivial), and aims at identifying the nonlinear map of an attracting manifold (in certain cases the stable manifold itself [55]), on the basis of which the slow process dynamics (once the fast transients die out) can be explicitly characterized. The two approaches could conceivably be used in tandem for model reduction purposes of complex chemical reaction systems.

Remark 2.5. The possibility of integrating the proposed approach into a nonlinear MPC synthesis framework certainly deserves further examination and traces a meaningful line of future research work. On an intuitive level, it is expected that nonlinear controller design based on the methodological principles of MPC for the process dynamics evolving on the stable slow manifold can be considerably simplified, and the associated on-line optimization problem become less computationally demanding due to the lower dimensionality of the problem under consideration.

2.3.1 Special Case: The Long-Term Dynamic Behavior of Linear Discrete-Time Processes

Let us now consider the special case of a linear (or linearized around a reference steady state (x^0, w^0)) discrete-time dynamic process model:

$$x(k+1) = Bx(k) + Cw(k) \tag{2.25}$$

where $x \in \mathbb{R}^n$ is the vector of process state variables, and for the sake of simplicity, let $w \in \mathbb{R}$ be a time-varying scalar process parameter following the first-order dynamics:

$$w(k+1) = aw(k) \tag{2.26}$$

with B,C being constant matrices with appropriate dimensions and $|a| < 1$ (stability assumption for the w-dynamics). Notice that one may envision a case where a chemical reaction system with z being the composition vector (in deviation form from the reference steady state conditions), and w the catalyst activity (in deviation form as well) corresponding to a specific deactivation mechanism, is modeled by (2.25)-(2.26) [32]. In this representative case, the objective is to calculate the long-term asymptotic behavior of the chemical reaction system (2.25) in the presence of catalyst deactivation (2.26), and therefore, to investigate the possibility of catalyst replacement if conversion or selectivity are affected in an adverse manner.

It is assumed that the eigenspectrum of the process characteristic matrix B is comprised of eigenvalues λ_i with $\lambda_i < 1, i = 1, ..., n$, and therefore the discrete-time process (2.25) is assumed to be a stable one. Notice, that in the case of an unstable process, one could assume that a stabilizing controller has been already synthetized to ensure closed-loop stability, and therefore, the previous stability assumption should not be viewed as a restrictive one within the context of the present study. Furthermore, it is assumed that the time-constant associated with the catalyst activity w-dynamics is larger compared to the dominant process time-constant:

$$|a| >> \rho \tag{2.27}$$

where $\rho = \max_i |\lambda_i|, (i = 1, ..., n)$ is the spectral radius of the process characteristic matrix B. Within the current context, this assumption appears to be valid and reasonable for chemical reaction systems where catalyst deactivation by poisoning occurs [32]. One may now explicitly calculate the long-term asymptotic process response in the presence of catalyst deactivation (2.26) through a direct computation of the solution $x(k)$ of the system of linear difference equations (2.25) and (2.26) [27]:

$$\begin{aligned} x(k) &= B^k x(0) + \sum_{i=0}^{k-1} B^{k-i-1} C a^i w(0) \\ &= B^k x(0) - w(0) \left\{ a^k I - B^k \right\} (B - aI)^{-1} C \end{aligned} \tag{2.28}$$

where the following matrix identity was used:

$$\sum_{j=0}^{k-1} B^{k-j-1} a^j = \left\{ B^k - a^k I \right\} (B - aI)^{-1} \tag{2.29}$$

Under assumption (2.27), it can be easily inferred that the longterm asymptotic response of the linear discrete-time process (2.25) in the presence of catalyst deactivation (2.26) is given by:

$$x(k) \underset{k \to \infty}{\approx} -w(0)(B - aI)^{-1} C a^k \tag{2.30}$$

It should be pointed out that the same expression for the long-term asymptotic process response can be derived by following the proposed approach which is based on the explicit construction of the invariant manifold S (2.9). Indeed, in the linear case (2.25) and (2.26), the associated system of invariance NFEs (2.5) takes the following form:

$$\begin{aligned} \pi(aw) &= B\pi(w) + Cw \\ \pi(0) &= 0 \end{aligned} \tag{2.31}$$

Under the assumptions of Theorem 2.1, the above system of NFEs admits a unique solution:

$$\pi(w) = \Pi w \tag{2.32}$$

where Π is the unique solution that satisfies the following Lyapunov matrix equation:

$$\Pi aI - B\Pi = C \tag{2.33}$$

It is easy to show that (2.33) admits the following solution:

$$\Pi = -(B - aI)^{-1}C \tag{2.34}$$

where $(B-aI)$ is indeed an invertible matrix since a does not belong to the eigenspectrum of the process characteristic matrix B, which is guaranteed by Lemma 2.1 and Theorem 2.1. According to Theorem 2.2, the invariant manifold $x = \Pi w$ is locally attractive, and the long-term asymptotic behavior of the chemical reaction system (2.25) in the presence of catalyst deactivation (2.26) is given by:

$$x(k) \underset{k\to\infty}{\approx} \Pi w(k) = -w(0)(B - aI)^{-1}Ca^k \tag{2.35}$$

The above expression was derived on the basis of the invariant manifold construction of the proposed approach, and it coincides with the one (Eq. (2.30)) obtained through a direct calculation of the solution of the discrete-time linear process dynamic equations (2.25) and (2.26). Notice that the proposed approach naturally reproduces the results offered by linear analysis, and it can be therefore viewed as its nonlinear analogue.

2.4 Illustrative example

Immobilized cell and enzyme bioreactors are now widely used in a variety of interesting applications. In these systems, the short-term behavior of the bioreactor is dependent upon the nonlinear kinetics of the immobilized enzymes or cells participating in the reactions. However, the long-term behavior of the bioreactors depends upon the stability of the immobilized enzymes or the viability of the immobilized cells. The short-term behavior of these systems is important in determining the conversion of a

nutraceutical or degradation of a toxin, for example, parameters that define the performance of the bioreactor. The long-term behavior of the bioreactor will determine when the enzyme or cell catalyst needs to be replaced in order to maintain conversions at acceptable levels. Therefore, accurately estimating when bioreactor performance declines below acceptable levels has important consequences for the profitability of a process or the health of a patient. Actual kinetic data on enzyme performance and enzyme degradation are considered in the present study for an immobilized enzyme bioreactor that is used for the production of food grade linoleic acid from corn oil [88]. In the case study considered, we assume that the enzymatic bioreactor behaves as an ideal continuous stirred tank reactor (CSTR). It is also assumed that the enzyme involved converts substrate into product, in this case corn oil into linoleic acid, via a pingpong bi-mechanism, as reported in [88]. Under a set of standard assumptions, the following nonlinear dynamic process model can be developed:

$$\begin{aligned} \frac{dS}{dt} &= f^{(1)}(S,E) = \frac{k_1 ES}{1-k_2 S} + \frac{v_0}{V}(S_0 - S) \\ \frac{dE}{dt} &= g^{(1)}(E) = -k_{d1} E \end{aligned} \tag{2.36}$$

Parameter	Value
S_0	$3.4M$
$S(t=0)$	$3M$
$E(t=0)$	$3g$
V	$50ml$
v_0	$100ml/h$
k_1	$8.2 \times 10^{-2} h^{-1} g^{-1}$
k_2	$5.9 \times 10^{-1} M^{-1}$
k_{d1}	$3.4 \times 10^{-3} h^{-1}$

Table 2: Kinetic and bioreactor parameter values

The above dynamic equations describe the change in substrate concentration in the reactor as a function of time, and the degradation of activity of the enzyme. S, S_0 and E represent the concentrations of substrate, substrate in the feed stream and enzyme, respectively. k_1 and k_2 represent kinetic parameters describing the rate of the

enzymatic reaction and k_{d1} is a kinetic parameter describing the rate of deactivation of the enzyme. v_0 is the flow rate of the substrate and V is the reactor volume. In Table 2, kinetic parameters used in the example, as well as initial substrate and enzyme concentrations, are provided. It is worth mentioning that under these parameter values, the above bioreactor dynamics is characterized by a latent two-time scale multiplicity attributed to the slow degradation of the enzyme when compared to the much faster bioprocess dynamics. Using a time-discretization step: $\delta = 0.01h$, which is smaller than the dominant process time-constant, Euler's discretization method was applied in order to obtain a quite accurate discrete-time dynamic process model (sampled-data representation of (2.36)):

$$\begin{array}{rclcl} S(k+1) & = & F^{(1)}(S(k),E(k)) & = & S(k)+f^{(1)}(S(k),E(k))\delta \\ E(k+1) & = & G^{(1)}(E(k)) & = & E(k)+g^{(1)}(E(k))\delta \end{array} \tag{2.37}$$

In order to conform to the theory presented in previous sections, the following set of deviation variables relative to the equilibrium point $(S_0, E_0) = (3.4, 0)$ is introduced:

$$\begin{array}{rcl} x & = & S - S^0 \\ w & = & E - E^0 \end{array} \tag{2.38}$$

Let us also denote: $\bar{F}^{(1)}(x,w) = F^{(1)}(x+S^0, w+E^0), \bar{G}^{(1)}(w) = G^{(1)}(, w+E^0)$. Notice that for the bioreactor model (2.37), all conditions of Theorems 2.1 and 2.2 are satisfied. Therefore, there exists a unique and locally analytic invariant manifold: $x = \pi(w)$, with $\pi(w)$ being the solution of the following nonlinear functional equation:

$$\begin{array}{c} \pi(\bar{G}^{(1)}(w)) = \bar{F}^{(1)}(\pi(w), w) \\ \pi(0) = 0 \end{array} \tag{2.39}$$

A series solution of the above functional equation is sought around the origin. The Taylor coefficients of the unknown solution $x = \pi(w)$ can be automatically computed by using a simple MAPLE code. A finite-order series truncation N is considered leading to a Taylor polynomial approximation $u = \pi^{[N]}(w)$ of the actual solution

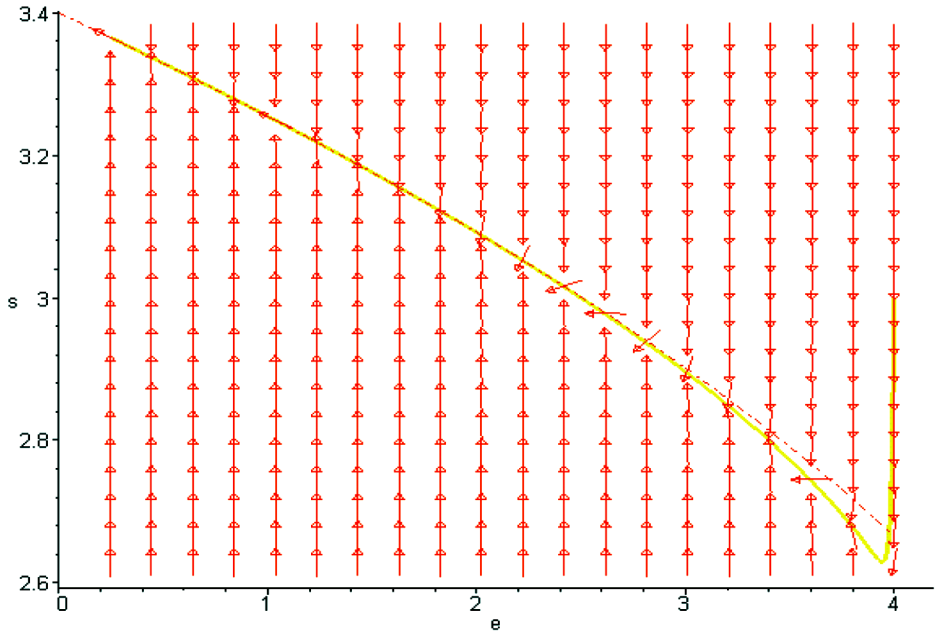

Figure 2.1: Phaseportrait of the bioreactor dynamics slow manifold ($N = 5$).

of the invariance nonlinear functional equation (2.39). In particular, with the aid of the aforementioned MAPLE code up to a 10th-order series truncation was considered: $N = 1, ..., 10$. Figs. 2.1 and 2.2 represent the phaseportrait of the bioreactor dynamics along with the actual slow invariant manifold (depicted through the solid line) and the one obtained through the solution of the invariance functional equation (2.39) for $N =$ 5 and 10, respectively (depicted through the dotted line). It should be first pointed out that the underlying two-time scale multiplicity manifests itself quite explicitly and the familiar dynamic pattern naturally emerges [64]: the transition of the system from the initial state to the slow manifold is depicted through the vertical constant-E lines since the enzymatic concentration remains practically unchanged due to the much slower enzymatic dynamics, while the substrate concentration changes rather rapidly until the system reaches the slow manifold, upon which the bioreactor dynamics is bound to evolve (for large times). Please notice the satisfactory approximation of the actual slow invariant manifold by the proposed method in the case of $N = 5$, and the almost indistinguishable curves in the $N = 10$ case. As intuitively expected and as a result

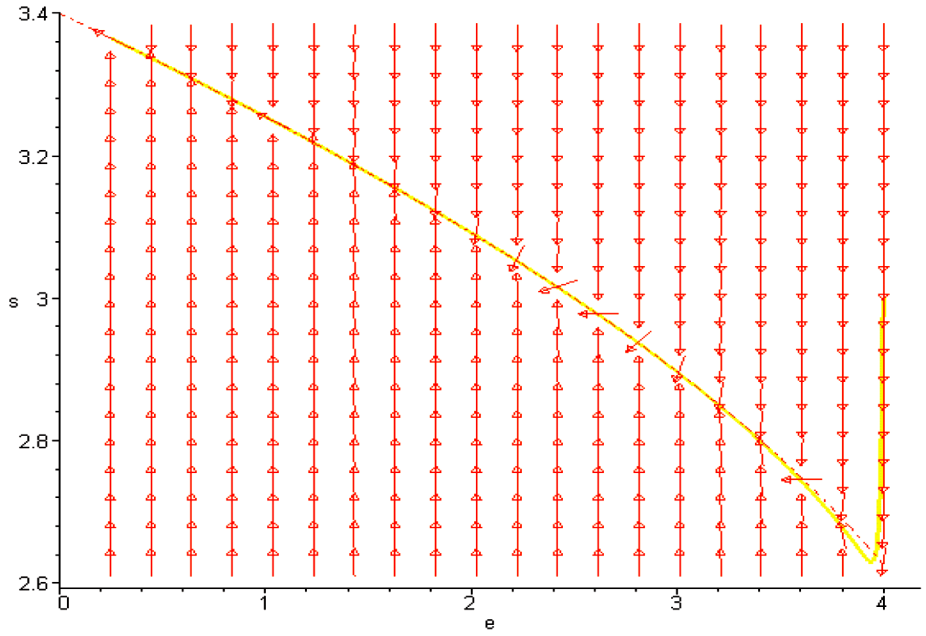

Figure 2.2: Phaseportrait of the bioreactor dynamics slow manifold ($N = 10$).

of the uniform convergence of the series solution of (2.39), numerical convergence to the actual slow invariant manifold can be satisfactorily demonstrated. Both the actual dynamic response of the bioreactor was computed by simulating the full process model (2.37), as well as the long-term asymptotic behavior of the bioreactor by using the proposed method and Eq. (2.24) with $N = 10$ and $u = \pi^{[10]}(w)$, a 10th-order Taylor polynomial approximation of the actual solution of the invariance functional equation (2.39). As it can be seen in Fig. 2.3, the estimated substrate concentration profile (dotted line) at the outlet of the reactor obtained through the proposed method becomes indistinguishable from the actual substrate concentration profile (solid line) at times larger than $100h$, which is less than the approximate half-life of the decaying enzyme. Fig. 2.4 shows the actual conversion profile (solid line) in the bioreactor as well as the conversion estimated (dotted line) from the asymptotic behavior of the bioreactor as characterized through the proposed method. Please notice that the proposed method accurately approximates the actual conversion profile, and therefore allows the satisfactory monitoring of the actual bioprocess performance, at times much

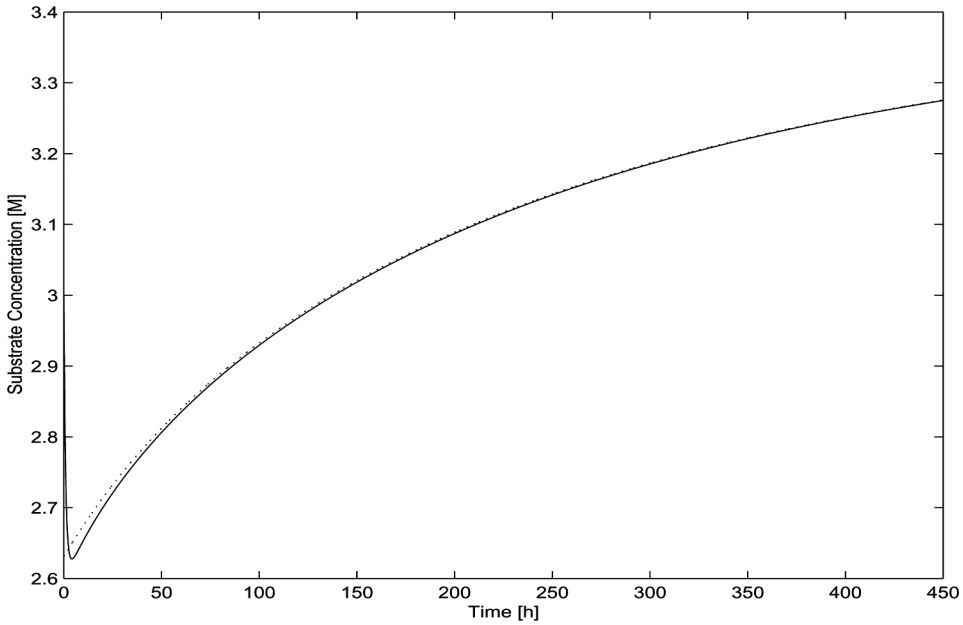

Figure 2.3: Comparison between the actual and estimated substrate concentration profiles ($N = 10$).

shorter than the half-life of the decaying enzyme.

2.5 Concluding remarks

A new approach to the problem of computing and quantitatively characterizing the long-term dynamic behavior of nonlinear discrete-time processes was presented. The formulation of the problem of interest was conveniently realized through a system of nonlinear functional equations for which a rather general set of conditions for the existence and uniqueness of a locally analytic solution was derived. The solution to the aforementioned system of NFEs was then shown to represent a locally analytic invariant manifold of the nonlinear discrete-time dynamic process model considered. The local analyticity property of the invariant manifold enabled the development of a series solution method, which can be easily implemented using a simple MAPLE code. Under a certain set of conditions, it was also shown that the invariant manifold computed attracts all system trajectories, and therefore, the asymptotic process response and long-term dynamic behavior can be explicitly determined through the

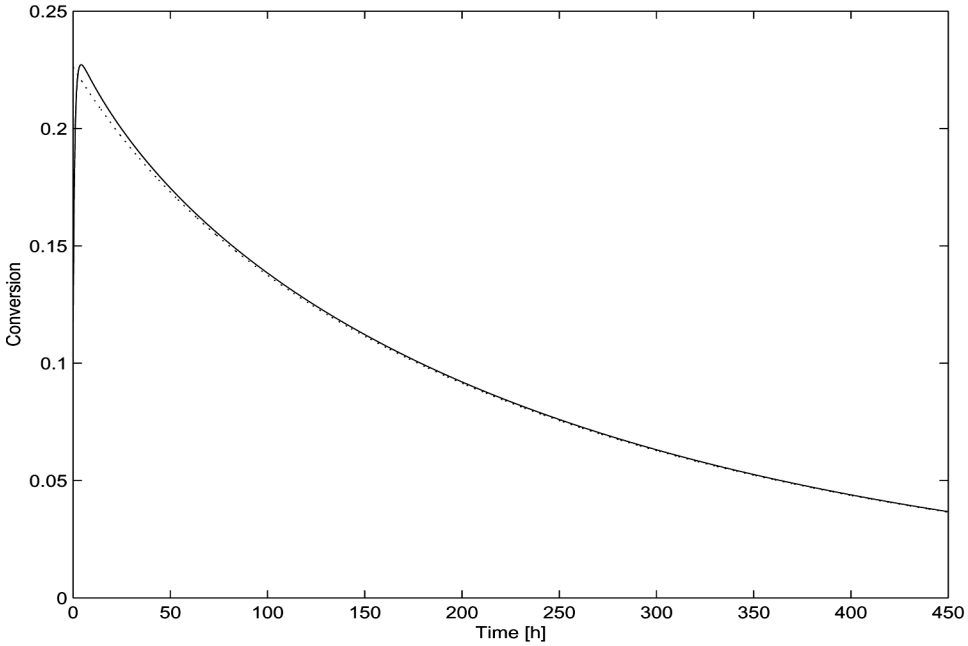

Figure 2.4: Comparison between the actual and estimated substrate conversion profiles ($N = 10$).

restriction of the discrete-time process dynamics on the invariant manifold.

CHAPTER 3

Nonlinear Observer Design for Process Monitoring in the Presence of Time-Scale Multiplicity

3.1 Introduction

The problem of the development of operationally flexible and reliable methods to accurately reconstruct the unmeasurable process state variables, as well as other key quantities associated with process safety and/or product quality, is of central importance in process control, monitoring and diagnostics [24, 92]. Indeed, technical limitations and cost-related considerations that affect segments of current sensor technology, as well as inherent physical limitations associated with the measurement of certain physical and/or chemical quantities, necessitate and motivate the development of methods that allow the accurate estimation of the above unmeasurable quantities [24, 92]. A widely followed strategy to accomplish this objective relies on the design of model-based state observers that make explicit use of the available process measurements and are capable of providing accurate estimates for the unmeasurable process state variables [24,92]. For linear processes, both the popular Kalman

filter [40] and its deterministic analogue known as the Luenberger observer [73], form the basis of a comprehensive and practically intuitive framework that adequately addresses the linear state estimation problem. However, the recognition that the majority of physical and/or chemical processes exhibit nonlinear behavior and the occasional difficulties encountered when linear observers are designed on the basis of linearized process models characterized of local validity [24, 92], induced a wave of research efforts aiming at developing the requisite nonlinear observer design methods that could directly cope with process nonlinearities. As a result, a number of notable nonlinear observer design frameworks emerged, where various methodological objectives were pursued and perspectives offered, as well as different aspects of the underlying state estimation problem emphasized [1,4,9,19,22,23,29,39,44,65–69,71,91,96]. However, all the above approaches presuppose the availability of a dynamic process model that does not exhibit time-scale multiplicity (a process dynamic response characteristic that naturally arises in a multitude of applications), and most importantly, the sensor dynamics is not integrated into their respective observer design frameworks, and thus its impact on the viability and performance of the proposed observer remains inevitably unaddressed. Please notice, that for processes exhibiting fast and slow dynamic modes (such as instrumented processes where there is a latent time-scale separation property that distinguishes the fast sensor dynamics from the slow process dynamics, as well as reactor networks and classes of bioprocesses that exhibit inherent time-scale multiplicity [14,16,70], the state estimation problem becomes not only theoretically challenging due to the multiple timescales, but practically an intriguing and important one [13, 62, 74]). Indeed, one could in principle realize the design of the nonlinear observer through the restriction of the process dynamics on the slow manifold (the reduced-order process dynamic model), and thus capitalizing on all the computational and analytical advantages that the lower-dimensionality of

the problem of interest brings, followed by a detailed, rigorous and insightful analysis on the impact of the ignored fast dynamics (otherwise known as parasitics) on the convergence properties of the reduced-order observer [62, 74]. It should be emphasized, that the design of nonlinear observers based on the reduced-order process dynamic model on the slow manifold is motivated by the fact that model-based estimation problems for systems/processes exhibiting time-scale multiplicity, and thus stiff dynamics, may lead to ill-conditioned observer gains and potentially undermine the convergence properties of an observer designed for the full-order singularly perturbed system (3.1) [16, 70]. Please notice that the aforementioned problem has been thoroughly studied for linear systems [49], and within a singular perturbation framework of analysis, pursued by a few researchers on the nonlinear front as well. In particular, high-gain [15, 26, 62, 74, 94] and sliding-mode observers [46] have been designed for special classes of nonlinear systems, that explicitly take into account the underlying time-scale separation property of the system under consideration, and nicely embedded it into their respective frameworks of analysis and design.

The present work [59], while adopting a singular perturbation framework of analysis, aims at developing a generic and systematic nonlinear observer design method for fast/slow systems, as well as overcoming some of the restrictions associated with the above approaches by following a methodologically and technically different path. In particular, a nonlinear observer is designed on the basis of the reduced order process dynamics evolving on the slow manifold, and the effect of the unmodeled fast component (which may represent the sensor dynamics in an overall dynamic description of an instrumented process) of the process dynamics on the estimation error dynamics is carefully analyzed and mathematically characterized. It is shown, that in the proposed method, the observer error generated by neglecting the fast process dynamics is of order $O(\epsilon)$, where ϵ is the perturbation parameter and a measure of the relative speed/time-constant of the fast and the slow component of the process

dynamics. Therefore, the proposed method establishes robustness of the observer design method with respect to fast unmodeled process dynamics.

The present Chapter is organized as follows: in Section 3.2 some mathematical preliminaries are presented, as well as the problem formulation. In Section 3.3 the Chapter's main results are provided, and a detailed analysis on the behavior of the estimation error induced by the proposed observer is performed in the presence of the unmodeled fast component of the process dynamics. Finally, some concluding remarks are provided in Section 3.5.

3.2 Mathematical preliminaries and problem formulation

In the context of the present study single-output nonlinear dynamic process models are considered, that are mathematically realized through the following standard singular perturbation state-space representation form:

$$\begin{aligned} \dot{x}(t) &= \frac{dx(t)}{dt} = f\left(x(t), w_(t)\right) \\ \epsilon\dot{w}(t) &= \epsilon\frac{dw(t)}{dt} = M_1(t)x(t) + M_2(t)w(t) \\ y(t) &= C_1x(t) + C_2w(t) \end{aligned} \tag{3.1}$$

where $x \in X \subset \mathbb{R}^n$ is the vector of the slow process state variables, $w \in W \subset \mathbb{R}^m$ is the vector of states associated with the fast w-dynamics and X,W are compact sets containing the origin, ϵ is the perturbation parameter that represents a measure of the relative speed/time-constant of the fast and the slow component of the overall process dynamics and through which the latent two-time-scale separation is explicitly quantified, and $y \in \mathbb{R}$ is the measured process output variable. It is assumed that $f(x, w)$ is a real analytic vector function defined on $X \times W$, and M_1, M_2, C_1, C_2 are constant matrices/ vectors of appropriate dimensions with M_2 being nonsingular. It should be pointed out, that the state-space representation (3.1) of a singularly perturbed

system with linear fast w-dynamics captures a broad class of interesting cases such as instrumented processes where the fast dynamics represent the sensor dynamics, biological processes, reactor networks, etc. [16, 70]. Furthermore, in numerous studies the fast component of the process dynamics is typically considered as unmodeled, and inevitably, robustness questions arise in relation to the design of model-based process control and observer-based monitoring systems [14, 16, 70]. Without loss of generality, it is assumed that system (3.1) is expressed in deviation variable form, so that the origin $(x, w) = (0, 0)$ is an equilibrium point of (3.1) with: $f(0, 0) = 0$. If one neglects the fast process dynamics by setting $\epsilon = 0$, the following reduced-order dynamical system represents the restriction of the process dynamics the slow manifold: $M_1 x + M_2 w = 0$ [63]:

$$\begin{aligned} \dot{\bar{x}}(t) &= \frac{d\bar{x}(t)}{dt} = \bar{f}\left(\bar{x}(t)\right) \\ \bar{y}(t) &= C_0 \bar{x}(t) \end{aligned} \tag{3.2}$$

where:

$$\begin{aligned} \bar{f}\left(\bar{x}\right) &= f\left(\bar{x}, -M_2^{-1} M_1 \bar{x}\right) \\ C_0 &= C_1 - C_2 M_2^{-1} M_1 \end{aligned} \tag{3.3}$$

Without considering the full system (3.1) and on the basis of the above reduced-order system (3.2) that represents the process dynamics on the slow manifold, the simplified design of an appropriate nonlinear observer could be in principle realized, and thus lead to estimates of the unmeasurable slow process state variables. The idea of designing nonlinear observers using the reduced-order process dynamics (3.2) on the low-dimensional slow manifold rather than the entire two-time-scale singularly perturbed system description (3.1), is motivated by the fact that the dynamics of system (3.1) is stiff, occasionally leading to ill-conditioned observer gains and structure (highly sensitive to the perturbation parameter ϵ), and adversely affecting the observer's convergence properties [16, 70]. However, neglecting the fast sensor dynamics will inevitably introduce an observer error, and therefore, a rigorous analysis

of its effect on the convergence properties of the proposed observer and the associated estimation error dynamics should be carefully performed. Another interesting way of addressing the estimation problem under consideration, is to consider the fast component of the process dynamics as unmodeled (e.g. unmodeled fast sensor dynamics), and conduct the requisite analysis on the robustness properties of the proposed reduced-order nonlinear observer design method on the system's slow manifold and in the presence of fast unmodeled process dynamics. The above considerations essentially dictate the main objectives and focus of the present research study. Within the proposed methodological framework, the point of departure is the reduced-order system (3.2), to which the principles of the nonlinear observer design methodology introduced in [60] are applied. According to the design method presented [60], one considers a nonlinear identity observer of the following form:

$$\dot{\hat{x}} = \bar{f}(\hat{x}) + L\left(\hat{x}\right)\left(y - \hat{y}\right) \tag{3.4}$$

where $\hat{x} \in \mathbb{R}^n$ is the state estimate, and $\hat{y} = C\hat{x}$. The above nonlinear observer has a state-dependent gain $L(x)$, which can be computed as follows:

$$L(x) = \left[\frac{\partial T}{\partial x}(x)\right]^{-1} B \tag{3.5}$$

where $T(\bar{x})\colon \mathbb{R}^n \to \mathbb{R}^n$ is a solution to the following associated system of first-order non-homogeneous linear partial differential equations (PDEs):

$$\frac{\partial T}{\partial \bar{x}} \bar{f}(\bar{x}) = AT\left(\bar{x}\right) + BC_0\bar{x} \tag{3.6}$$

with A, B being constant matrices of appropriate dimensions. Under the above choice of the nonlinear gain and in the absence of sensor dynamics, the observer (3.4) induces linear error dynamics in the transformed coordinates $\bar{z} = T(\bar{x})$ for the reduced-order

process model (3.2) [60]:

$$\begin{aligned}
\frac{de}{dt} &= \frac{d}{dt}(\bar{z}-\hat{z}) = \frac{d}{dt}(T(\bar{x})-T(\hat{x})) = \frac{\partial T}{\partial \bar{x}}\frac{d\bar{x}}{dt} - \frac{\partial T}{\partial \hat{x}}\frac{d\hat{x}}{dt} \\
&= \frac{\partial T}{\partial \bar{x}}\bar{f}(\bar{x}) - \frac{\partial T}{\partial \hat{x}}\frac{d\hat{x}}{dt}\left\{\bar{f}(\hat{x}) + L(\hat{x})(y - C\hat{x})\right\} \\
&= AT(\bar{x}) + \cancel{BC_0\bar{x}} - AT(\hat{x}) - \cancel{BC_0\hat{x}} - \cancel{BC_0\bar{x}} + \cancel{BC_0\hat{x}} \Longrightarrow \\
\frac{de}{dt} &= A(T(\bar{x})-T(\hat{x})) = A(\bar{z}-\hat{z}) = Ae
\end{aligned} \tag{3.7}$$

and therefore, if A is chosen to be Hurwitz, its eigenvalues regulate the exponential rate of decay of the estimation error $(T(\bar{x}) - T(\hat{x}))$ to zero. Notice, that invertibility of the matrix $\dfrac{\partial T}{\partial \bar{x}}(\bar{x})$ (or the transformation map $T(\bar{x})$) implies that the state estimate $\hat{x}$ asymptotically approaches the actual state $\bar{x}$ [60].

Remark 3.1. To ensure the feasibility and viability of the observer (3.4), a set of necessary and sufficient conditions needs to be derived, under which the associated system of PDEs (3.6) admits a unique and invertible solution. Please notice, that in this case the proposed nonlinear observer (3.4) would exhibit the desirable convergence properties, or equivalently, it would generate state estimates that asymptotically converge to the actual unmeasurable states in the absence of fast w-dynamics. Furthermore, and from a practical point of view, the use of the observer (3.4) requires the development of a comprehensive solution method for the system of PDEs (3.6). 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 $\bar{f}_i(\bar{x})(k = 1, ..., n)$ of the vector function $\bar{f}(\bar{x})$ [20, 60]. Furthermore, notice that the principal part vanishes at $\bar{x} = 0$ due to the equilibrium condition, and thus, the origin becomes a characteristic (singular) point for the system of PDEs (3.6) [20, 60]. 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 first-order PDEs (3.6) [20], and inevitably one needs to resort to methods and results from singular PDE theory [60]. Indeed, it can

be proven that under a set of rather generic necessary and sufficient conditions the above system of singular PDEs (3.6) admits a unique locally analytic and invertible solution in the neighborhood of the reference equilibrium point $\bar{x} = 0$ (see Appendix B); for detailed proofs see [60,68,69]. Furthermore, the unknown solution's analyticity property enables the development of a comprehensive and practical solution method for the system of PDEs (3.6) as delineated in Appendix B.

In the presence of the fast w-dynamics one can easily show that, within the above nonlinear observer design framework, the estimation error dynamics is no longer linearizable, and one needs to be prepared to encounter an inevitable observer error whose behavior and impact on the estimation error dynamics needs to be assessed and quantified. Indeed, in this case the estimation error dynamics can be calculated in the following fashion:

$$\begin{aligned}
\frac{de}{dt} &= \frac{d}{dt}(z-\hat{z}) = \frac{d}{dt}(T(x)-T(\hat{x})) = \frac{\partial T}{\partial x}\frac{dx}{dt} - \frac{\partial T}{\partial \hat{x}}\frac{d\hat{x}}{dt} \\
&= \frac{\partial T}{\partial x} f(x,w) - \frac{\partial T}{\partial \hat{x}}\left\{\bar{f}(\hat{x}) + L(\hat{x})(y - C_0\hat{x})\right\} \\
&= \frac{\partial T}{\partial x} f(x,w) - \frac{\partial T}{\partial \hat{x}}\bar{f}(\hat{x}) - B\left(C_1 x + C_2 w - C_0\hat{x}\right) \\
&= \frac{\partial T}{\partial x} f(x,w) - \frac{\partial T}{\partial x}\bar{f}(x) + \frac{\partial T}{\partial x}\bar{f}(x) \\
&\quad -\frac{\partial T}{\partial \hat{x}}\bar{f}(\hat{x}) - B\left(C_1 x + C_2 w - C_0\hat{x}\right) \\
&= A(T(x)-T(\hat{x})) - BC_2M_2^{-1}M_1 x - BC_2 w + \frac{\partial T}{\partial x} f(x,w) - \frac{\partial T}{\partial x}\bar{f}(x) \\
&= Ae - BC_2M_2^{-1}M_1 x - BC_2 w + \frac{\partial T}{\partial x} f(x,w) - \frac{\partial T}{\partial x}\bar{f}(x) \qquad (3.8)
\end{aligned}$$

From the above expression for the estimation error dynamics (3.8), it can be easily inferred that the proposed nonlinear observer (3.4) which was designed on the basis of the reduced order process dynamics (3.2) on the slow manifold does not induce linear error dynamics in the presence of the unmodeled fast process dynamics, its convergence properties are directly affected by the latter, and as intuitively expected, an observer error emerges even in the case of a zero observer initialization error. In

the ensuing theoretical developments and within the technical framework of singular perturbation theory, the inevitable observer error that arises due to the presence of the unmodeled fast dynamics will be analyzed and shown to be of order $O(\epsilon)$.

Within the standard singular perturbation context of analysis and sensor modeling framework, it is typical to invoke the assumption that matrix M_2 appearing in the sensor dynamic equations is Hurwitz (and thus invertible) [13,49,63,74]. Furthermore, in order to ensure closeness of solutions in the infinite time interval of the singularly perturbed system (3.1), local exponential stability of the reduced-order dynamics (3.2) is needed as well [17, 63]. An immediate consequence is that the mismatch: $\|w(t) - \bar{w}(t)\|$ between the sensor's true state w and the state $\bar{w}$ associated with the reduced-order dynamics (3.2) (the quasi-steady-state approximant): $\bar{w}(t) = -M_2^{-1}M_1\bar{x}(t)$, asymptotically decays with time-constants (dynamic modes) of the order of $O(\epsilon)$ [49, 63, 74]. The following technical lemma is essential for the ensuing theoretical developments:

Lemma 3.1. *Under the stated assumptions, one can show that [49, 63]:*

$$w(t) = \exp\left(\frac{M_2(t-t_0)}{\epsilon}\right)\left\{w(t_0) + M_2^{-1}M_1x(t_0)\right\} - M_2^{-1}M_1x(t) + O(\epsilon) \tag{3.9}$$

$\forall t \in [t_0, \infty)$*, where* t_0 *is the initial time instant.*

Using the result of Lemma 3.1, Eq. (3.8) becomes:

$$\begin{aligned}
\frac{de}{dt} &= Ae - BC_2M_2^{-1}M_1x - BC_2\left\{exp\left(\frac{M_2(t-t_0}{\epsilon}\right)\right. \\
&\quad \left.\times(w(t_0) + M_2^{-1}M_1x(t_0)) - M_2^{-1}M_1x(t)\right\} \\
&\quad + \frac{\partial T}{\partial x}f(x,w) - \frac{\partial T}{\partial x}\bar{f}(x) + O(\epsilon) \\
\frac{de}{dt} &= Ae - BC_2\left(exp\left(\frac{M_2(t-t_0)}{\epsilon}\right)(w(t_0) + M_2^{-1}M_1x(t_0))\right) \\
&\quad + \frac{\partial T}{\partial x}f(x,w) - \frac{\partial T}{\partial x}\bar{f}(x) + O(\epsilon)
\end{aligned} \tag{3.10}$$

From (3.10) it can be inferred that the estimation error satisfies the equation

below:

$$\begin{aligned} e(t) &= \exp(A(t-t_0))e(t_0) - \int_{t_0}^{t} exp(A(t-\bar{t})) \\ &\quad \times BC_2 exp\left(\frac{M_2(\bar{t}-t_0}{\epsilon}\right)(w(t_0)+M_2^{-1}M_1x(t_0))d\bar{t} \\ &\quad + \int_{t_0}^{t} exp\left(\frac{M_2(\bar{t}-t_0}{\epsilon}\right)\left(\frac{\partial T}{\partial x}(x(\bar{t}))f(x(\bar{t}),w(\bar{t})) - \frac{\partial T}{\partial x}(x(\bar{t}))\bar{f}(x(\bar{t}))\right)d\bar{t} \\ &\quad + O(\epsilon) \end{aligned} \tag{3.11}$$

where $e(t_0)$ represents the observer initialization error.

3.3 Main results

The following theorem captures the present chapter's main results.

Theorem 3.1. *For the original singularly perturbed system (3.1) and in the presence of locally asymptotically stable fast w-dynamics and locally exponentially stable reduced-order dynamics (3.2), the estimation error $e(t)$ that is induced by the observer (3.4) satisfies the following equation:*

$$e(t) = \exp\left(A(t-t_0)\right)e(t_0) + H(t,\epsilon) \tag{3.12}$$

where the observer error term $H(t,\epsilon)$ is of order $O(\epsilon)$ in $t \in [t_0, \infty)$.

Proof of Theorem 3.1. In Eq. (3.11), let us denote:

$$\begin{aligned} H_1(t,\epsilon) &= \int_{t_0}^{t} \exp(A(t-\tilde{t}))BC_2 \exp\left(\frac{M_2(\bar{t}-t_0)}{\epsilon}\right) \\ &\quad \left\{w(t_0)+M_2^{-1}M_1x(t_0)\right\}d\bar{t} \end{aligned} \tag{3.13}$$

and:

$$\begin{aligned} H_2(t,\epsilon) &= \int_{t_0}^{t} \exp(A(t-\bar{t}))\left\{\frac{\partial T}{\partial x}(x(\bar{t}))f(x(\bar{t}),w(\tilde{t}))\right. \\ &\quad \left. -\frac{\partial T}{\partial x}(x(\bar{t}))\bar{f}(x(\bar{t}))\right\}d\bar{t} \end{aligned} \tag{3.14}$$

For the function $H_1(t,\epsilon)$ one obtains:

$$\begin{aligned}\|H_1(t,\epsilon)\| &\leq \int_{t_0}^{t} \|exp(A(t-\bar{t}))\|\|BC_2\| \\ &\quad \times \left\|exp\frac{M_2(\bar{t}-t_0)}{\epsilon}\right\| \|w(t_0)+M_2^{-1}M_1x(t_0)\|d\bar{t} \\ &\leq \|BC_2\|\|w(t_0)+M_2^{-1}M_1x(t_0)\| \\ &\quad \times \int_{t_0}^{t} \|exp(A(t-\bar{t}))\| \left\|exp\left(\frac{M_2(\bar{t}-t_0}{\epsilon}\right)\right\| d\bar{t} \end{aligned} \tag{3.15}$$

Since both matrices A and M_2 are Hurwitz, there exist positive constants k_0, a_0, k_1, a_1 such that [63]:

$$\left\|\exp\left(\frac{M_2(\bar{t}-t_0)}{\epsilon}\right)\right\| \leq k_1 1 \exp\left(-\frac{a_1(\bar{t}-t_0)}{\epsilon}\right) \tag{3.16}$$

and:

$$\|\exp\left(A(t-\bar{t})\right)\| \leq k_0 \exp\left(-a_0(t-\bar{t})\right) \tag{3.17}$$

Therefore, Eq. (3.15) yields:

$$\begin{aligned}\|H_1(t,\epsilon)\| &\leq \frac{\epsilon k_0 k_1}{a_1-\epsilon a_0}\|BC_2\|\left\|w(t_0)+M_2^{-1}M_1x(t_0)\right\| \\ &\quad \times \left\{\exp(-a_0(t-t_0)) - \exp\left(-\frac{a_1(t-t_0)}{\epsilon}\right)\right\} \end{aligned} \tag{3.18}$$

Let us now establish a bound for the second term $H_2(t,\epsilon)$ in Eq. (3.11). Using (3.17) one obtains:

$$\begin{aligned}\|H_2(t,\epsilon)\| &\leq \int_{t_0}^{t} \|\exp(A(t-\bar{t}))\| \left\|\frac{\partial T}{\partial x}(x(\bar{t}))\right\| \\ &\quad \times \left\|f(x(\bar{t}),w(\tilde{t})) - \bar{f}(x(\bar{t}))\right\| d\bar{t} \\ &\leq k_0 \int_{t_0}^{t} \|\exp(-a_0(t-\bar{t}))\| \left\|\frac{\partial T}{\partial x}(x(\bar{t}))\right\| \\ &\quad \times \left\|f(x(\bar{t}),w(\bar{t})) - \bar{f}(x(\bar{t}))\right\| d\bar{t} \end{aligned} \tag{3.19}$$

The analyticity of the map $T(x)$ on the compact domain X, implies that there exists a positive constant L such that: $\dfrac{\partial T}{\partial x} \leq L$, for all $x \in X$. Furthermore, if we denote by y the "off-manifold" coordinate: $y(t) = w(t) - (M_2^{-1}M_1x(t)) = w(t) + M_2^{-1}M_1x(t)$, then the boundary layer system [63] for the original singularly

perturbed system (3.1) can be easily shown that it follows the linear dynamics below :

$$\frac{dy}{d\tau} = M_1 x + M_2(y - M_2^{-1}M_1 x) = M_2 y \tag{3.20}$$

where $\tau = t/\epsilon$ represents the fast time scale. Therefore, in light of (3.16) and (3.20) the following inequality can be established :

$$\|y(\tau)\| = \left\| y\left(\frac{t}{\epsilon}\right) \right\| \leq k_2 \exp\left(-\frac{a_1(t-t_0)}{\epsilon}\right) \tag{3.21}$$

where k_2 is a positive constant.

Under the assumptions stated and as a consequence of Tikhonov's theorem for the infinite time interval case, it can be inferred that the mismatch between the solution to the boundary-layer system dynamics (3.20) and $y(t)$ that are associated with the full fast/slow original system (3.1) is of order $O(\epsilon_i)$ ([63]):

$$y(t) - y\left(\frac{t}{\epsilon}\right) = y(t) - y(\tau) = O(\epsilon) \tag{3.22}$$

and furthermore, the following bound can be established for all $i \in [\![1, \ell]\!]$ [63]:

$$\|y(t)\| \leq k_2 \exp\left(-\frac{a_1(t-t_0)}{\epsilon}\right) + \epsilon\delta \tag{3.23}$$

with δ being a positive constant. Let us now denote:

$$F(x, y) = f(x, y - M_2^{-1}M_1 x) \tag{3.24}$$

One obtains:

$$\begin{aligned} \|f(x,w) - \bar{f}(x)\| &= \|f(x, y - M_2^{-1}M_1 x) \\ &\quad -f(x, -M_2^{-1}M_1 x)\| \\ &= \|F(x,y) - F(x,0)\| \end{aligned} \tag{3.25}$$

The analyticity of the vector function $F(x, y)$ on the compact domain of its definition, entails that there exist positive constants L_1 such that [63]:

$$\begin{aligned} \|F(x(\bar{t}), y(\bar{t})) - F(x(\bar{t}, 0))\| &\leq L_1\|y(\bar{t})\| \\ &\leq L_1\epsilon\delta + L_1 k_2 \exp\left(-\frac{a_1(\bar{t}-t_0)}{\epsilon}\right) \end{aligned} \tag{3.26}$$

due to Eq. (3.23).In light of (3.26), Eq. (3.19) yields:

$$\begin{aligned}\|H_2(t,\epsilon)\| &\leq \int_{t_0}^{t} k_0 \exp(-a_0(t-\bar{t})) \\ &\quad \times \left\{ LL_1\epsilon\delta + LL_1k_2 \exp\left(-\frac{a_1(\bar{t}-t_0)}{\epsilon}\right)\right\} d\bar{t} \\ &\leq k_0L\epsilon \left\{ \frac{L_1\delta}{a_0}(1-exp(-a_0(t-t_0))) \right. \\ &\quad \left. + \frac{L_1k_2}{a_1-\epsilon a_0}\left(exp(-a_0(t-t_0)) - exp\left(-\frac{a_1(t-t_0)}{\epsilon}\right)\right)\right\} \quad (3.27)\end{aligned}$$

On the basis of the derived bounds for the two nonlinear functions $H_1(t,\epsilon)$ and $H2(t,\epsilon)$, the following bound can be readily established for $H(t,\epsilon) \leq -H_1(t,\epsilon) + H_2(t,\epsilon)$:

$$\begin{aligned}\|H(t,\epsilon)\| &\leq \|H_1(t,\epsilon)\| + \|H_2(t,\epsilon)\| \\ &\leq \epsilon\left\{K_1 + K_2\exp(-a_0(t-t_0)) + K_3 exp\left(-\frac{a_1(t-t_0)}{\epsilon}\right)\right\} \quad (3.28)\end{aligned}$$

with:

$$\begin{aligned}K_1 &= \frac{k_0LL1\delta}{a_0} \\ K_2 &= \frac{k_0LL1k2}{a_1-\epsilon a_0} - \frac{k_0LL_1\delta}{a_0} + \frac{k_0k1}{a_1-\epsilon a_0}\|BC_2\|\|w(t_0) + M_2^{-1}M_1x(t_0)\| \\ K_3 &= -\frac{k_0k_1}{a_1-\epsilon a_0}\|BC_2\|\|w(t_0) + M_2^{-1}M_1x(t_0)\| - \frac{k_0LL_1k_2}{a_1-\epsilon a_0}\end{aligned}$$

Please notice that both K_2, K_3 are of order $O(1)$ with respect to the perturbation parameter ϵ, and therefore, the observer error term $H(t,\epsilon)$ is of order $O(\epsilon)$ due to (1.27), and the proof is complete. □

The following remarks are important in order to interpret the result of Theorem 3.1 and gain some insight into its practical consequences on the state estimation problem under consideration.

Remark 3.2.

Theorem 3.1 suggests that even in the absence of an observer initialization error ($e(t_0) = 0$), the proposed observer, which was designed on the basis of the reduce-dorder dynamic process model (3.2) on the slow manifold, generates state estimates that exhibit an inevitable estimation error when compared to the actual slow process state variables. However, this observer error has been shown to be of order $O(\epsilon)$. Therefore, the faster the unmodeled w-dynamics compared to the process dynamics (or equivalently, the smaller its time-constant compared to the fastest process time-constant), the less significant the observer error generated. Please notice that the result of Theorem 1 lends itself to the following interpretation as well:

(i) it establishes a concrete robustness property characterizing the proposed nonlinear observer design method against fast stable unmodeled process dynamics, and

(ii) it gives rise to a systematic reduced-order nonlinear observer design methodology that is realized on the systems low-dimensional slow manifold, thus effectively overcoming the occasionally ill-conditioned nature of an observer design based on the full-order singularly perturbed system (3.1) that exhibits stiff dynamics in a variety of practical applications [16, 70].

Remark 3.3. The established bound on the observer error $H(t, \epsilon)$ in Theorem 3.1, implies that it is of order $O(\epsilon)$ and consists of two time-varying terms of physical significance: a relatively slower exponentially decaying mode $\exp(-a_0(t-t_0))$ associated with the observer matrix A that enforces the requisite convergence speed of the slow state estimates to the actual process states, and the faster exponentially decaying dynamic modes $\exp(-a_1(t - t_0)/\epsilon)$ with time-constant of order $O(\epsilon)$ related to the unmodeled fast dynamics.

Remark 3.4. The proposed method can be generalized to a system with multiple-time-scale (more than two) of the type:

$$
\begin{aligned}
&\dot{x}(t) = \frac{dx(t)}{dt} = f\left(x(t), w_1(t), w_2(t), ..., w_\ell(t)\right) \\
&\begin{cases}
\epsilon_1 \dot{w}_1(t) &= \epsilon_1 \dfrac{dw_1(t)}{dt} &= M_1 x(t) + N_1 w_1(t) \\
\epsilon_2 \dot{w}_2(t) &= \epsilon_2 \dfrac{dw_2(t)}{dt} &= M_2 x(t) + N_2 w_2(t) \\
\vdots & \vdots & \vdots \\
\epsilon_\ell \dot{w}_\ell(t) &= \epsilon_\ell \dfrac{dw_\ell(t)}{dt} &= M_\ell x(t) + N_\ell w_\ell(t)
\end{cases} \\
&y(t) = C_0 x(t) + \textstyle\sum_{i=1}^{\ell} C_i w_i(t)
\end{aligned}
\tag{3.29}
$$

where: $x \in X \subset \mathbb{R}^n$ is the vector of the slow process state variables, $\ell \in \mathbb{N}$ is the number of independent fast dynamics. For all $i \in [\![1, \ell]\!]$:

- $w_i \in W_i \subset \mathbb{R}^m$is the vector of states associated with the ith fast dynamics
- X, Wi are compact sets containing the origin
- ϵ_i is the perturbation parameter that represents a measure of the relative speed/time-constant of the fast and the slow component of the overall process dynamics and through which the latent two-time-scale separation is explicitly quantified

and $y \in \mathbb{R}$ is the measured process output variable. It is assumed that $f(x, w_1, ..., w_\ell)$ is a real analytic vector function defined on $X \times W_1 \times .... \times W_\ell$, and for all $i \in [\![1, \ell]\!]$, M_i, N_i, C_i are constant matrices/vectors of appropriate dimensions with N_i being nonsingular.

The construction of the observer is very similar, based on the slow manifold created by setting $\forall i \in [\![1, \ell]\!]$ $\epsilon_i = 0$:

$$
\begin{cases}
M_1 x + N_1 w_1 = 0 \\
\vdots \\
M_i x + N_i w_i = 0
\end{cases}
\tag{3.30}
$$

and the reduced-order dynamical system represents the restriction of the process

dynamics on this slow manifold is expressed by [63]:

$$\begin{aligned} \dot{\bar{x}}(t) &= \tfrac{d\bar{x}}{dt} = \bar{f}\left(\bar{x}(t)\right) \\ \bar{y}(t) &= C\bar{x}(t) \end{aligned} \tag{3.31}$$

where:

$$\begin{aligned} \bar{f}\left(\bar{x}\right) &= f\left(\bar{x}, -N_1^{-1}M_1\bar{x}, -N_2^{-1}M_2\bar{x}, ..., -N_\ell^{-1}M_\ell\bar{x}\right) \\ C &= C_0 - \sum_{i=1}^{\ell} C_i N_i^{-1} M_i \end{aligned}$$

It can be shown that again the error generated by neglecting the fast process dynamics is of order $O(\epsilon)$, where ϵ is the greatest of the perturbation parameters ϵ_i.

3.4 Illustrative example

A typical continuous stirred-tank biological reactor is considered, where cells are being grown through the consumption of a substrate. Under the assumption of constant volume, the following dynamic process model can be developed [7]:

$$\begin{aligned} \dot{X} &= \frac{dX}{dt} = \mu(X,S)X - \frac{F}{V}X \\ \dot{S} &= \frac{dS}{dt} = -\frac{\mu(X,S)X}{Y} + \frac{F}{V}(S_F - S) \end{aligned} \tag{3.32}$$

where X, S are the cell-mass and substrate concentrations respectively, $\mu(X,S)$ is the specific growth rate, Y is the yield coefficient, F is the feedrate of the substrate, S_F is the feed concentration and V is the reactor volume. Under the assumption of Contois kinetics the specific growth rate takes the form [7, 39]:

$$\mu(X,S) = \frac{K_1 S}{K_2 X + S} \tag{3.33}$$

where K_1, K_2 are kinetic constants, and therefore, the process dynamic model 3.32 assumes the following form:

$$\begin{aligned} \dot{X} &= \frac{K_1 X S}{K_2 X + S} - \frac{F}{V}X \\ \dot{S} &= -\frac{K_1 X S}{K_2 X + S} + \frac{F}{V}(S_F - S) \end{aligned} \tag{3.34}$$

If we denote: $x_1 = X$, $x_2 = S$ and assign the following values to the model parameters: $K_1 = 1min^{-1}$, $K_2 = 1$, $Y = 1$, $F/V = 0.08min^{-1}$, $S_F = 0.1kg \cdot m^{-3}$, the following reactor model is obtained:

$$\begin{aligned} \dot{x}_1 &= \frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_1}{60} \\ \dot{x}_2 &= -\frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_2}{60} + \frac{0.008}{60} \end{aligned} \tag{3.35}$$

Please notice that the equilibrium point is $(x_{1,0}, x_{2,0}) = (0.092, 0.008)$. Current sensor technology allows the on-line measurement of the cell-mass concentration [25], and the associated sensor dynamics can be represented as follows [14, 25]:

$$\epsilon \dot{w} = \epsilon \frac{dw}{dt} = x_1 - w \tag{3.36}$$

where w is the state of the sensor dynamics, ϵ is its time constant that is considered as the perturbation parameter in the context of the present case study, and $y(t) = w(t)$ is the available sensor measurement. The objective is to estimate the substrate concentration $\hat{x}_2(t)$, by using the on-line sensor measurements for the cell-mass concentration $y(t) = w(t)$ [25]. According to the methodology presented in Section 3.3, the following observer is used, whose design was performed by neglecting the fast sensor dynamics:

$$\begin{aligned} \dot{\hat{x}}_1 &= \frac{\hat{x}_1 \hat{x}_2}{60(\hat{x}_1 + \hat{x}_2)} - \frac{0.08 \hat{x}_1}{60} + L_1(\hat{x}_1, \hat{x}_2)(y - \hat{x}_1) \\ \dot{\hat{x}}_2 &= -\frac{\hat{x}_1 \hat{x}_2}{60(\hat{x}_1 + \hat{x}_2)} - \frac{0.08 \hat{x}_2}{60} + \frac{0.008}{60} + L_2(\hat{x}_1, \hat{x}_2)(y - \hat{x}_1) \end{aligned} \tag{3.37}$$

where the nonlinear observer gain: $L(x) = [L1(x)|L2(x)]^T = \left[\frac{\partial T}{\partial x}(x)\right]^{-1}$ is computed through the following system of first-order singular PDEs:

$$\begin{aligned} &\frac{\partial T_1}{\partial x_1}\left(\frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_1}{60}\right) + \frac{\partial T_1}{\partial x_2}\left(-\frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_2}{60} + \frac{0.008}{60}\right) \\ &\qquad = a_{11} T_1 + a_{12} T_2 + b_1 x_1 \\ &\frac{\partial T_2}{\partial x_1}\left(\frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_1}{60}\right) + \frac{\partial T_2}{\partial x_2}\left(-\frac{x_1 x_2}{60(x_1 + x_2)} - \frac{0.08 x_2}{60} + \frac{0.008}{60}\right) \\ &\qquad = a_{12} T_1 + a_{22} T_2 + b_2 x_1 \end{aligned} \tag{3.38}$$

$$T_1(x_{1,0}, x_{2,0}) = T_1(0.092, 0.008) = 0$$

$$T_2(x_{1,0}, x_{2,0}) = T_2(0.092, 0.008) = 0$$

In the present case study, the following design parameters have been selected:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} -0.1 & 0 \\ 0 & -0.2 \end{bmatrix} \tag{3.39}$$

and:

$$B = \begin{bmatrix} b_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \tag{3.40}$$

Under the above choice of design parameters, the system of singular PDEs (3.38) admits a unique locally analytic and invertible solution $w = T(x)$, since all conditions presented in Appendix B are satisfied. A series solution of the above system of PDEs (3.38) 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 $w = T(x)$ are automatically computed by using a simple MAPLE code. In particular, a third-order truncation $w = T^{[3]}(x_1, x_2)$ of the Taylor series expansion of $w = T(x_1, x_2)$ is considered and given by:

$$\begin{aligned} w_1 &= T_1^{[3]}(x_1, x_2) \qquad (3.41) \\ &= 10.1224(x_1 - 0.092) - 1.6887(x_2 - 0.008) \\ &\quad +0.1254(x_1 - 0.092)^2 - 3.4561(x_1 - 0.092) \\ &\quad (x2 - 0.008) + 29.8104(x^2 - 0.008)^2 \\ &\quad -1.2314(x^1 - 0.092)3 + 32.0972(x_1 - 0.092)^2 \\ &\quad \times(x_2 - 0.008) - 191.0671(x_1 - 0.092) \\ &\quad \times(x_2 - 0.008)2 - 399.6450(x_2 - 0.008)^3 \\ &\quad +O(|x_1 - 0.092|^4, |x_2 - 0.008|^4) \end{aligned}$$

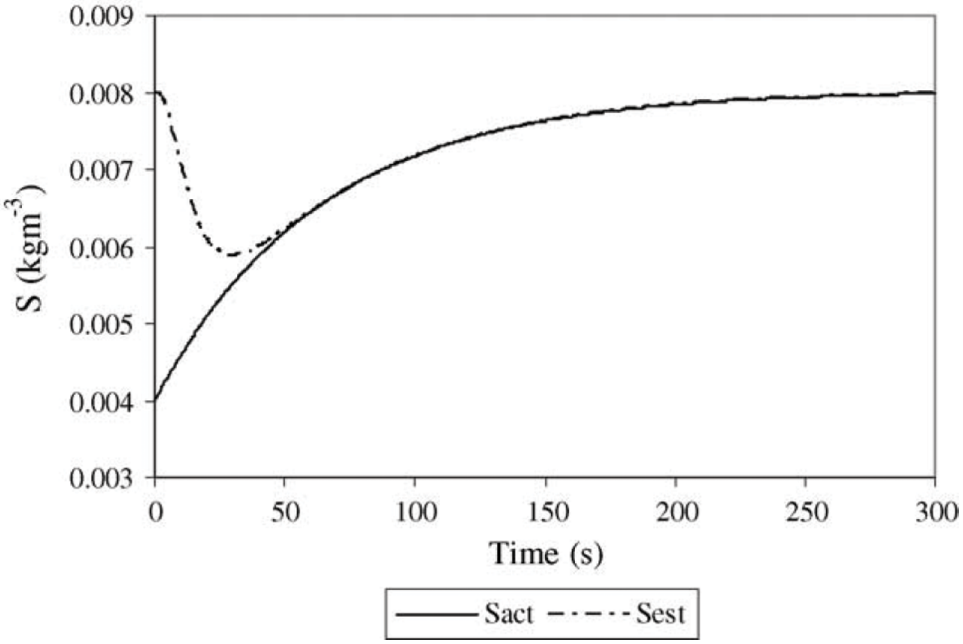

Figure 3.1: Estimation of substrate concentration for $\epsilon = 2\%$ of the fastest process time-constant.

$$
\begin{aligned}
w_2 &= T_2^{[3]}(x_1, x_2) && (3.42)\\
&= 10.0613(x_1 - 0.092) - 0.7690(x_2 - 0.008)\\
&\quad +0.0572(x_1 - 0.092)^2 - 1.4475(x_1 - 0.092)\\
&\quad \times(x_2 - 0.008) + 9.1546(x_2 - 0.008)2\\
&\quad -1.7181(x_1 - 0.092)^3 + 13.6812(x_1 - 0.092)2\\
&\quad \times(x_2 - 0.008) - 73.4817(x_1 - 0.092)(x_2 - 0.008)2\\
&\quad -110.8042(x_2 - 0.008)^3\\
&\quad +O(|x_1 - 0.092|^4, |x_2 - 0.008|^4) && (3.43)
\end{aligned}
$$

On the basis of the above third-order polynomial approximation $w = T^{[3]}(x_1, x_2)$ of the actual solution $w = T(x_1, x_2)$ of the system of PDEs (3.38) the proposed nonlinear observer (3.37) was simulated for different values of the perturbation parameter ϵ. The impact of sensor dynamics on the performance and convergence properties of the observer (3.38) is shown in Figs. 3.1, 3.2 and 3.3. The time-constant of the sensor

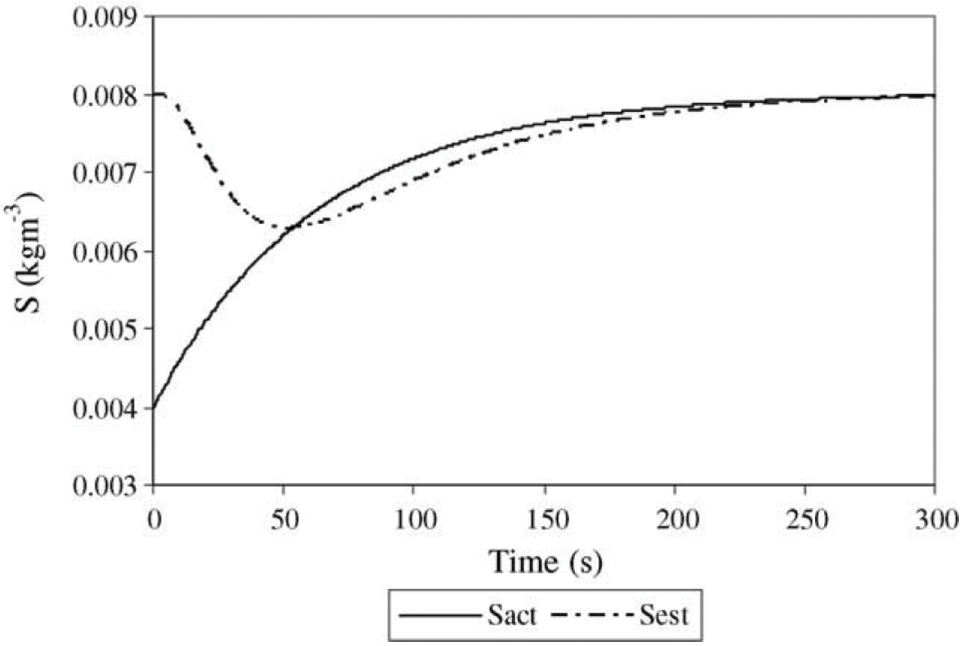

Figure 3.2: Estimation of substrate concentration for $\epsilon = 30\%$ of the fastest process time-constant.

dynamics is 2% of the fastest process time-constant in Fig. 3.1. In this case, the sensor dynamics is fast enough, that there is virtually no impact on the performance of the observer, which is quite satisfactory. In Fig. 3.2, the time-constant of the sensor dynamics is 30% of the fastest process time constant. At this value, there is a noticeable impact on the observer's performance, as the estimate responds slower and undershoots the actual process state. Please notice, that the observer state (estimate) still converges to the actual process state,yet not as quickly as in Fig. 3.1. In Fig. 3.3, the time constant of the sensor dynamics is almost comparable to the fastest process time-constant. As it can be inferred, the convergence is obviously much slower, and the inevitable observer error much greater. However, with sensor dynamics this slow and clearly not negligible (the singular perturbation framework of analysis is no longer adequate), one needs to consider it part of the overall (instrumented) process model, on the basis of which a higher-order observer that explicitly takes it into account should be designed.

3.5 Concluding remarks

A new approach to the nonlinear observer design problem in the presence of multiple time-scales was presented. The design of the proposed nonlinear observer was realized through the reduced-order process dynamics that evolve on the system's slow manifold. Furthermore, the behavior of the estimation error that the proposed nonlinear observer induces in the presence of unmodeled fast process dynamics was carefully analyzed, and within a singular perturbation framework of analysis, was shown to be of order $O(\epsilon)$, where ϵ is the slowest perturbation parameter and a measure of the relative speed/time-constant of the fast and the slow component of the process dynamics. Therefore, the analysis conducted established robustness of the proposed observer design method with respect to fast unmodeled process dynamics. Finally, it should be pointed out that the proposed observer design method could in principle be integrated into the output feedback controller synthesis framework for multiple-time-scale processes introduced in [18], tracing a meaningful future research direction.

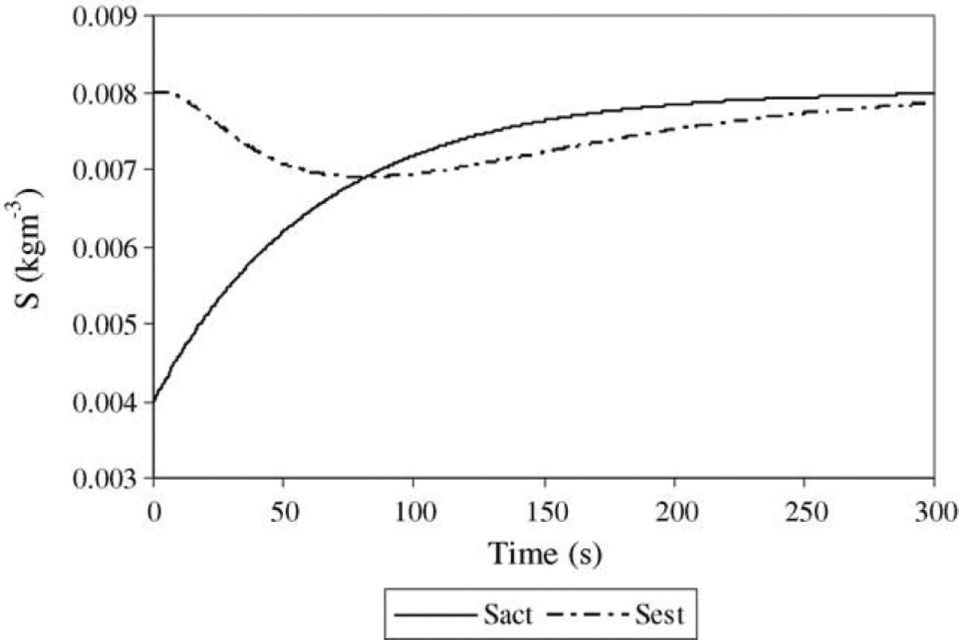

Figure 3.3: Estimation of substrate concentration for ϵ comparable in magnitude to the fastest process time-constant.

CHAPTER 4

Discrete-time Nonlinear Observer Design for Chemical Reaction Systems in the Presence of Model Uncertainty

4.1 Introduction

Broad classes of chemical reaction systems exhibit nonlinear dynamic behavior and are typically modeled by systems of nonlinear differential equations [28, 76, 87]. These dynamic models aim at capturing the actual behavior of the system of interest as faithfully 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.) [5, 7, 18, 36, 53, 76, 85–87, 90] . 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 [7, 18, 36]. 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 [24, 92]. 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 [7, 18, 24, 92]]. 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 [48, 92]. 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 [40] and its deterministic analogue realized by Luenberger's observer [12, 73], 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 [40, 92]. However, this approach exhibits only local validity because it overlooks the dominant process nonlinearities, and as reported in [40], 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 [48]. 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 [7, 40]. Undoubtedly, the first systematic approaches for the development of a design method for nonlinear observers were reported in [9, 66, 67], 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 [48]. Other important contributions to the nonlinear observer design problem can be found in [2, 4, 19, 23, 39, 44, 50, 69, 91, 96] , 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 can not 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 [7, 15, 18]. It is therefore quite important to investigate the possibility of designing observers that are capable of providing robust and accurate estimates of the unmeasurable quantities in the presence of model uncertainty and/or modeling errors [15, 18].

The development of such an observer, which should be able to overcome the model uncertainties, requires online measurement of some specific measured states through a sensor. From a practical point of view, the online measurement is realized through computer acquisition cards, which involve a sampling of the analog signal sent by the sensor. The use of a continuous-time nonlinear observer is therefore practically difficult to realize, and one should consider the realization of a discrete-time nonlinear observer.

This chapter is organized as follows: In section 2, the necessary mathematical prerequisites are briefly presented. Section 3 is reporting the main results and section 4 will include some concluding remarks.

4.2 Mathematical preliminaries and problem formulation

Let us consider spatially homogeneous chemical reactions systems, which can be described by the M chemical reactions involving S species:

$$\sum_{j=1}^{S} \nu_{ij} A_j \rightleftharpoons 0 \tag{4.1}$$

where $i = 1, \ldots, M$ and ν_{ij} denotes the stoichiometric coefficients of the j-th species A_j in the i reaction. It is assumed that the reactions are taking place in a standard continuous stirred-tank reactor (CSTR) and that the volume of the reacting mixture remains constant [36, 87]. Let us denote r_i and ΔH_i the reaction rate and the heat of chemical reaction number i, respectively. By applying mass and energy balances, one can derive the dynamics of the considered reactions as a system of nonlinear ordinary differential equations (ODEs) which describes the evolution of the various species concentrations, and the reacting mixture temperature inside the reactor [36, 97]:

$$\begin{aligned} \frac{dC_j}{dt} &= \sum_{i=1}^{M} \nu_{ij} r_i + \frac{F}{\rho V}\left(C_j^{in} - C_j\right), \\ \frac{dT}{dt} &= -\frac{1}{\rho C_p} \sum_{i=1}^{M} \Delta H_i r_i + \frac{F C_p^{in}}{\rho V C_p}\left(T^{in} - T\right) + \frac{UA}{\rho V C_p}\left(T^h - T\right). \end{aligned} \tag{4.2}$$

where C_j represents 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. A more compact mathematical representation of the system (4.2) can be realized through the

use of vectorial/matrix notations, by defining the vector of variables:

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

often called the state vector (or vector of state variables), because it uniquely determines and characterizes the dynamic of the reaction system (4.1), since its evolution is deterministically governed by the system of ODEs (4.2) [41, 43, 95]. Let us also define:

(i) the M-dimensional reaction rate vector:

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

where each reaction rate r_i associated to the reaction i is expressed as : $r_i = k_i(T)\tilde{r}_i(C)$, with $k_i(T)$ being the temperature-dependent kinetic rate constant [36, 97].

(ii) the $(S+1) \times M$-dimensional generalized stoichiometric matrix [97]:

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

(iii) the vector function: $J(x)$, $J\colon R^{S+1} \rightarrow R^{S+1}$ containing all remaining terms in

the system of ODEs (4.2) associated with mass flow and heat transfer [36, 97]:

$$J(x) = \begin{bmatrix} \frac{F}{\rho V}\left(C_1^{in} - C_1\right) \\ \vdots \\ \frac{F}{\rho V}\left(C_S^{in} - C_S\right) \\ \frac{FC_P^{in}}{\rho V C_p}\left(T^{in} - T\right) + \frac{UA}{\rho V C_p}\left(T^h - T\right) \end{bmatrix}.$$

The use of the vectorial/matrix notations provides us with the following form fo system (4.2):

$$\frac{dx(t)}{dt} = N\left(x(t)\right) r\left(x(t)\right) + J\left(x(t)\right) \equiv F\left(x(t)\right), \tag{4.3}$$

where $F(x), F\colon R^{S+1} \rightarrow R^{S+1}$ denotes the vector function on the right hand-side of ODEs (4.3). Furthermore, for the present study, it is assumed that $x \in X \subset R^{S+1}$, where X is a compact subset of the state space (in other words, it is implicitly assumed that the dynamical system (4.3) is stable with bounded space trajectories $x(t)$ contained in X or that a controller has been synthesized to render the controlled reaction system stable) and $F(x)$ is a real analytic vector function on X. Without loss of generality, it can be assumed that the origin $x_0 = 0$ is an equilibrium point of (4.3). Indeed, if the equilibrium point is non-zero, the following linear transformation $\tilde{x} = x - x_0$ with $\tilde{F}(\tilde{x}) \equiv F(\tilde{x} + x^0)$ maps the non-zero equilibrium point x_0 to the origin in the new system of coordinates, where the system's dynamics is represented as follows:

$$\frac{d\tilde{x}(t)}{dt} = \tilde{F}\left(\tilde{x}(t)\right). \tag{4.4}$$

For convenience purposes, the notation used in (4.3) will be used in the rest of the study. The aim of the study being to design a digital state estimator or observer, a discretization method [18, 28, 78] is used to obtain a discrete-time system of the following form (typically called a sampled-data represention of (4.4)) :

$$x(k+1) = \Phi\left(x(k)\right), \tag{4.5}$$

where $k \in \mathbb{N}$ is the discrete-time index and $\Phi\colon R^{S+1} \rightarrow R^{S+1}$. In practice, this discrete-time dynamic model often does not capture faithfully the behavior of the actual system over all possible regimes because of the presence of model uncertainty. For example, certain parameters of the model, like the kinetic parameters in the present study could be unknown or approximated and as such, they add uncertainty to the model of the system [7, 18, 36, 87, 92]. This uncertainty can be represented mathematically as follows:

$$x(k+1) = \Phi\left(x(k)\right) = \varphi\left(x(k)\right) + \varepsilon\gamma\left(x(k)\right), \tag{4.6}$$

where the vector function $x(k+1) = \Phi\left(x(k)\right)$ is now partitioned into two terms: $\Phi\left(x(k)\right) = \varphi\left(x(k)\right) + \varepsilon\gamma\left(x(k)\right)$. $\varphi\left(x(k)\right)$, with $\phi\left(\left(x(0)\right)\right) = 0$ is the known part (or equivalently the nominal part) of the dynamical model and $\varepsilon\gamma\left(x(k)\right)$ represents the model uncertainty or modeling error. It should be noticed that $\varepsilon > 0$ represents usually a small number (perturbation parameter) and even though $\gamma\left(x(k)\right)$ is not exactly determined, it is not entirely unknown, in the sense that it could be bounded in some way. Indeed, it is often assumed that the term $\gamma\left(x(k)\right)$ is bounded on X and satisfies the following condition:

$$\|\gamma(x(k))\| \leq M, \tag{4.7}$$

where $M > 0$ and $x \in X$. Let us now introduce the online measurements used for the state reconstruction. The $m < (S+1)$ quantities y_i are available for direct on-line measurement, and can be represented mathematically as functions of the state variables: $y \in R^m$, $y = [y_1, \ldots, y_m] = \eta\left(x(k)\right)$, where $\eta\colon R^{S+1} \rightarrow R^m$ is a real analytic vector function. Very often y is a subset of the state variables and are measured using available sensor technology: $y = [x_1, \ldots, x_m]$, whereas the rest $(S+1-m)$ variables: $[x_{m+1}, \ldots, x_{S+1}]$ are unmeasurable. The purpose of this study is to accurately reconstruct these unmeasurable states in order to ensure product quality, process safety and/or performance monitoring. It is for example easily conceivable

that a temperature or a pressure measurement can be obtained faster and more reliably than a concentration. Similarly a cell mass concentration in a biochemical reaction is easier to measure than a substrate or enzyme concentration [7, 18, 24, 36, 87, 92]. Considering the known discrete-time nominal dynamic model and the sensor measurement signal:

$$\begin{aligned} x(k+1) &= \varphi\left(x(k)\right) \\ y(k) &= \eta\left(x(k)\right). \end{aligned} \tag{4.8}$$

one can design a digital observer :

$$\hat{x}(k+1) = \omega\left(\hat{x}(k), y(k)\right) \tag{4.9}$$

which is also a discrete dynamical system itself, driven by the on-line sensor measurements $y(k)$ and capable of providing accurate estimates $\hat{x}(k)$ of the actual state vector $x(k)$, in the sense that the estimation error: $e(k) = x(k) - \hat{x}(k)$ (or the mismatch between the state x and its estimate $\hat{x}$) converges to zero asymptotically: $\|e(k)\| = \|x(k) - \hat{x}(k)\| \to 0$, as $k \to \infty$. Consequently, the convergence properties of the state estimator or observer are determined by the appropriate choice of the vector function $\omega\left(\hat{x}, y\right)$ on the right-hand side of the observer's dynamic equations (4.9).This choice should cause the estimation error $e(k)$ to decay over time, and preferably provide stable, smooth and fast dynamic modes to the estimation error dynamics. In other words the choice of the vector function $\omega\left(\hat{x}, y\right)$ must be dictated by the desired speed/rate of convergence of the state estimate $\hat{x}$ to the actual state x. After presenting this observer, a question comes naturally to mind: Would this observer still offer a reliable state vector estimate $\hat{x}$ that converges to the actual state x in the presence of the model uncertainty $\gamma(x)$, and therefore would the convergence properties be robust to modeling error and uncertainty? Mathematically stated, what are the conditions that render the estimation error dynamics structurally stable in the presence of the perturbation term $\varepsilon\gamma(x)$, or equivalently, is the stability of the error dynamics robust

in the presence of model uncertainty or error? The next section will be dedicated to the study of this problem.

4.3 Main results

From a methodological point of view, it is necessary for us to start by studying the state estimator design for the unperturbed system (4.8) as presented in [60]. This first step will form the basic framework of analysis, and will be adapted to the later robustness properties study. The design of the state estimator for the nominal unperturbed system is realized as follows. Let us suppose that there exists a change of state coordinates $z = \theta(x)$, $\theta \colon R^{S+1} \rightarrow R^{S+1}$, an output injection term $\beta(y)$ and an $(S+1) \times (S+1)$ matrix A such that the dynamics of the system (4.6) in the z-coordinates is linear and driven by the nonlinear output injection term $\beta(y)$: $z(k+1) = Az(k) + \beta\left(y(k)\right)$. Then, $\theta(x)$ should satisfy the following system of first order functional equations (FEs):

$$\begin{aligned} \theta(\varphi(x)) &= A\theta(x) + \beta(\eta(x)) \\ \theta(0) &= 0, \end{aligned} \tag{4.10}$$

Using this change of coordinates, the following observer can be constructed:

$$\begin{aligned} \hat{z}(k+1) &= A\hat{z}(k) + \beta\left(y(k)\right) \\ \hat{x}(k) &= \theta^{-1}\left(\hat{z}(k)\right). \end{aligned} \tag{4.11}$$

In the original coordinates system, it can be shown that the observer becomes:

$$\hat{x}\left(k+1\right) = \theta^{-1}\left[\theta\left(\varphi\left(\hat{x}(k)\right)\right) + \beta\left(y(k)\right) - \beta\left(h\left(\hat{x}(k)\right)\right)\right]. \tag{4.12}$$

In this case corresponding to the nominal system (4.8), the following error dynamics can be derived in the transformed coordinates $z = \theta(x)$:

$$\begin{aligned} e_z(k+1) &= z(k+1) - \hat{z}(k+1) \\ &= Az(k) + \cancel{\beta\left(y(k)\right)} - A\hat{z}(k) - \cancel{\beta\left(y(k)\right)} \Longrightarrow \\ e_z(k+1) &= Ae_z(k). \end{aligned} \tag{4.13}$$

The above error dynamics is linear and if the fundamental matrix A is chosen to have stable eigenvalues, these eigenvalues will regulate the decay of the estimation error $e_z(k) = z(k) - \hat{z}(k)$ to zero (eigenmodes of the estimation error dynamics (4.13)). Moreover the invertibility of $\theta(x)$ ensures that the state estimates $\hat{x}$ asymptotically converge to the actual state x. A set of necessary and sufficient conditions need to be determined in order to ensure the feasibility of the observer design (4.11). Particularly the associated system of FEs (4.10) must admit a unique and invertible solution. This is provided by [60] under a set of rather generic necessary and sufficient conditions, under which the system of FEs (4.10) admits a unique and locally analytic and invertible solution in the neighborhood of the equilibrium point. However, from a practical point of view, in order to use the observer (4.11) the development of a solution method for the system of FEs (4.10) is required. As mentioned previously the functions $\varphi(x)$, $\eta(x)$, and $\theta(x)$ are all locally analytic. It is therefore possible to expand $\varphi(x)$, $\eta(x)$, and the unknown solution $\theta(x)$ in multivariate Taylor series. Using these series expansion in the system of FEs (4.10) and equating the Taylor coefficients on both sides, recursion algebraic formulas are generated. These formulas are linear with respect to the Taylor coefficients of the unknown solution. Consequently, one can express the N-th order Taylor coefficients of $\theta(x)$ as a function of the Taylor coefficient up to the order $N-1$, which are calculated in previous steps. To simplify these recursive formulas , tensorial notation can be used. In particular, as defined in [60] , the following notational rules 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 derivative of the μ-th component $\varphi_\mu(x)$ of a vector field $\varphi(x)$ at $x = 0$ are denoted as follows:

$$\varphi^i_\mu = \frac{\partial \varphi_\mu}{\partial x_i}(0), \quad \varphi^{ij}_\mu = \frac{\partial^2 \varphi_\mu}{\partial x_i \partial x_j}(0), \quad \varphi^{ijk}_\mu = \frac{\partial^3 \varphi_\mu}{\partial x_i \partial x_j \partial x_k}(0),$$

etc.

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

One can notice that using the above notational convention, the l-th component $\theta_l(x)$ of the unknown solution $\theta(x)$ of the system of FEs (4.10) can be rewritten in a multivariate Taylor series form in the following fashion:

$$\theta_l(x) = \frac{1}{1!}\theta^{i_1}_l x_{i_1} + \frac{1}{2!}\theta^{i_1 i_2}_l x_{i_1} x_{i_2} + \ldots + \frac{1}{N!}\theta^{i_1 i_2 \ldots i_N}_l x_{i_1} x_{i_2} \ldots x_{i_N} + \ldots . \tag{4.14}$$

The functions $\varphi(x)$ and $\eta(x)$ are similarly expanded in Taylor series, and then inserted into FEs (4.10). Matching the coefficients of the same order, the following recursion formulas for the N-th order Taylor coefficients of the unknown solution $\theta(x)$ [60]:

$$\sum_{L=1}^{N-1} \sum_{0 \le m_1 \le m_2 \le \ldots \le m_L} \theta^{j_1 \ldots j_L}_l \varphi^{m_1}_1 \ldots \varphi^{m_L}_L = a^\mu_l \theta^{i_1 \ldots i_N}_\mu + b^\mu_l \theta^{i_1 \ldots i_N}_\mu, \tag{4.15}$$

where $m_1 + m_2 + \ldots + m_L = N$, $i_1, \ldots, i_N = 1, \ldots, n$. Notice that (4.15) represents a set of linear algebraic equations in the unknown coefficients $\theta^{i_1 \ldots i_N}_\mu$, and consequently a symbolic software package like MAPLE can be used to solve a simple code, developped that automatically provides the Taylor cofficients of the unknown solution of (4.10) .

Remark 4.1. The state observer (4.11) is based on the explicit construction of an

invariant manifold map $z = \theta(x)$ for the system:

$$\begin{aligned} x(k+1) &= \varphi\left(x(k)\right) \\ z(k+1) &= Az(k) + \beta(\eta\left(x(k)\right)), \end{aligned} \tag{4.16}$$

This augmented system contains both the original nominal dynamical system (4.8) and the observer dynamics expressed in the transformed coordinates. One can indeed show that the invariance requirement is translated into the system of invariance FEs (4.10) [41,43,55,86,95,99]. Also, it should be pointed out that the augmented system (4.15) belongs to the class of the so-called skew-product systems [89]: the original system dynamics driving the state observer dynamics through the sampled sensor measurement $y(k) = \eta(x(k)))$ as shown in (4.15). At this point let us determine how the convergence properties of the state observer (4.11) is affected in the presence of the model uncertainty or modeling error $\gamma(x)$. Particularly from a mathematical point of view, it is of interest to determine whether or not the estimation error dynamics associated with the state observer (4.11) remains structurally stable in the presence of the model uncertainty $\gamma(x)$. As it has been shown earlier, the observer (4.11) based on the nominal model (4.8) produces linear error dynamics with assignable rate of decay shown in (4.13). However, the introduction of the model uncertainty $\gamma(x)$ induces the following estimation error dynamics in the transformed coordinates $e_z = z - \hat{z}$:

$$
\begin{aligned}
e_z(k+1) &= z(k+1) - \hat{z}(k+1) \\
&= \theta\left[x(k+1)\right] - \theta\left[\hat{x}(k+1)\right] \\
&= \theta\left[\varphi(x(k)) + \varepsilon\gamma(x(k))\right] \\
&\quad -\theta\left\{\theta^{-1}\left[\theta(\varphi(\hat{x}(k)) + \beta(y(k)) - \beta(\eta(x(k)))\right]\right\} \\
&= \theta\left[\varphi(x(k)) + \varepsilon\gamma(x(k))\right] \\
&\quad -\theta(\varphi(\hat{x}(k)) - \beta(y(k)) + \beta(\eta(x(k))) \\
&\approx \theta\left[\varphi(x(k))\right] + \frac{\partial\theta}{\partial x}\gamma(x(k))\varepsilon \\
&\quad -\theta(\varphi(\hat{x}(k)) - \beta(y(k)) + \beta(\eta(x(k))) \\
&\approx A\theta(x(k)) + \cancel{\beta(\eta(x(k)))} + \frac{\partial\theta}{\partial x}\gamma(x(k))\varepsilon \\
&\quad -A\theta(\hat{x}(k)) - \cancel{\beta(\eta(\hat{x}(k)))} - \cancel{\beta(\eta(x(k)))} + \cancel{\beta(\eta(\hat{x}(k)))} \Longrightarrow \\
e_z(k+1) &\approx Ae_z(k) + \varepsilon\frac{\partial\theta}{\partial x}\gamma(x(k)). \qquad (4.17)
\end{aligned}
$$

The above error dynamics is obviously not linear anymore. It is composed of a linear term, corresponding to the nominal dynamical system, and a nonlinear term $\varepsilon\frac{\partial\theta}{\partial x}\gamma(x(k))$ introduced by the model uncertainty. In particular, the linear part represents a linear dynamical system with a stable fundamental matrix A, chosen to correspond to the desired observer design (4.11). Equation (4.17) yields [27]:

$$
e_z(k) = A^k e_z(0) + \sum_{j=0}^{k-1} A^{k-j-1}\frac{\partial\theta}{\partial x}(x(j))\gamma(x(j))\varepsilon. \qquad (4.18)
$$

Since A has stable eigenvalues, there exist positive constants $\alpha \in (0,1)$, $\delta > 0$ such that for all $y \in \mathbb{R}^{S+1}$ [11, 27]:

$$
\|A^k y\| \leq \delta(\alpha)^k \|y\|, \qquad (4.19)
$$

and the estimation error can be bounded as follows:

$$\begin{aligned}
\|e_z(k)\| &\leq \delta(\alpha)^k\|e_z(0)\| + \varepsilon\sum_{j=0}^{k-1}\delta\alpha^{k-j-1}\left\|\frac{\partial\theta}{\partial x}(x(j))\right\|\|\gamma(x(j))\| \\
&\leq \delta(\alpha)^k\|e_z(0)\| + \varepsilon\delta LM\sum_{j=0}^{k-1}\alpha^{k-j-1} \\
\|e_z(k)\| &\leq \delta(\alpha)^k\|e_z(0)\| + \varepsilon\delta LM\frac{1-\alpha^k}{1-\alpha}, \qquad (4.20)
\end{aligned}$$

where $e_z(0)$ is the initial estimation error of the unmeasurable states and $\|\partial\theta/\partial x\| \leq L$ in the compact set X. Result (4.20) yields the following important remarks:

(i) Without model uncertainty: $\gamma(x) \equiv 0$, the estimation error in the transformed coordinates converges to zero: $\|e_z(k)\| = \|\hat{z}(k) - z(k)\| \to 0$, as $k \to \infty$. Invoking the analyticity and local invertibility property of the coordinate transformation map $z = \theta(x)$, it can be established that the estimation error expressed in the original coordinates converges to zero as well: $\|e(k)\| = \|\hat{x}(k) - x(k)\| \to 0$, as $k \to \infty$.

(ii) In the presence of the model uncertainty term $\gamma(x)$ the estimation error does not converge asymptotically to zero even in the presence of zero initial estimation error: $e_z(0) = 0$. However (4.20) shows that the offset is of order $O(\varepsilon)$. In other words, the estimation error will be ultimately bounded by a small bound of the same order of magnitude as the model uncertainty term:

$$\begin{aligned}
\|e_z\| \qquad &\leq \qquad \frac{\epsilon\delta LM}{1-\alpha} \qquad (4.21) \\
&(k \to \infty)
\end{aligned}$$

4.4 Concluding remarks

In this chapter a new approach to the observer design problem in discrete-time is proposed for nonlinear chemical reaction systems in the presence of model uncertainty.

Specifically the observer dynamic equations are derived through the solution of a system of FEs, and the convergence properties of the estimation error dynamics were analyzed and quantitatively analyzed in the presence of model uncertainty.

CHAPTER 5

Conclusions

The first Chapter aimed at the development of a systematic method to optimally choose the parameters of digitally controlled nonlinear reactor dynamics. In addition to traditional performance requirements for the controlled reactor dynamics such as stability, fast and smooth regulation, disturbance rejection, etc., optimality was requested with respect to a physically meaningful performance index. The value of the performance index is analytically calculated via the solution of a Zubov-like functional equation and became explicitly parameterized by the digital controller parameters. A standard static optimization algorithm yielded subsequently the optimal values of the above parameters. Within the proposed framework, stability region estimates were provided through the solution of the above functional equation. Finally, a nonlinear chemical reactor example following Van de Vusse kinetics was used in order to illustrate the proposed parametric optimization method.

It should be pointed out, that the proposed method could be refined with the use of a dedicated programming language, which would increase the computational efficiency by integrating the symbolic solution of the Zubov-like functional equation with the above static optimization problem.

The second Chapter proposed a new approach to the problem of quantitatively

characterizing the long-term dynamic behavior of nonlinear discrete-time processes. It was assumed that in order to analyze the process dynamic behavior and digitally simulate it for performance monitoring purposes, the discrete-time dynamic process model considered could be obtained: (i) either through the employment of efficient and accurate discretization methods for the original continuous-time process which is mathematically described by a system of nonlinear ordinary (ODEs) or partial differential equations (PDEs) or (ii) through direct identification methods. In particular, nonlinear processes were considered whose dynamics can be viewed as driven: (i) either by an external time-varying forcing input/disturbance term, (ii) by a set of time-varying process parameters or (iii) by the autonomous dynamics of an upstream process. The formulation of the problem of interest was realized through a system of nonlinear functional equations (NFEs), for which a rather general set of conditions for the existence and uniqueness of a solution was derived. The solution to the aforementioned system of NFEs was then proven to represent a locally analytic invariant manifold of the nonlinear discrete-time process under consideration. The local analyticity property of the invariant manifold map enables the development of a series solution method for the above system of NFEs, which was implemented with the aid of a symbolic software package such as MAPLE. Under a certain set of conditions, it was shown that the invariant manifold computed attracts all system trajectories, and therefore, the asymptotic process response and long-term dynamic behavior were determined through the restriction of the discrete-time process dynamics on the invariant manifold. An illustrative case study of an enzymatic bioreactor was presented.

The problem considered in this chapter could be extended by considering w-dynamics that would be dependent on the state variable x. This would broaden the field of applications of the proposed method. One could for example consider the problem of a concentration-dependent catalyst deactivation mechanism, which would

be more representative of the actual catalyst deactivation.

The third Chapter presented a new approach to the nonlinear observer design problem in the presence of two-time-scale multiplicity. In particular, nonlinear processes were considered that exhibit fast and unmeasurable slow dynamic modes, and the latter needed to be accurately reconstructed through the use of a state observer. The proposed observer was designed on the basis of the reduced-order process dynamics that evolve on the system's slow manifold, and the dynamic behavior of the estimation error is analyzed and mathematically characterized in the presence of the unmodeled fast process dynamics. It was shown, that within the proposed nonlinear observer design framework, the observation error generated by neglecting the fast process dynamics was of order $O(\epsilon)$, where ϵ was the perturbation parameter and a measure of the relative speed/time-constant of the fast and the slow component of the process dynamics. Furthermore, the analysis conducted established robustness of the proposed observer design method with respect to fast unmodeled process dynamics. Finally, the performance of the proposed method and the convergence properties of the reduced-order nonlinear observer designed were evaluated in an illustrative biological reactor example.

As a future research direction, this problem could be adapted within a more general framework than the explicit standard singular perturbation problem considered in the present Thesis. One could for example consider the case of unmodeled perturbations or non-singular perturbation analysis.

In the fourth Chapter, a new solution to the unmeasurable state reconstruction problem in discrete-time for nonlinear chemical reaction systems in the presence of

model uncertainty was proposed. In particular, a new robust nonlinear state estimation method was 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 was conveniently formulated and addressed within the context of nonlinear functional equations (NFEs) theory, leading to a discrete-time nonlinear state estimator that possesses a state-dependent gain computed through the solution of a system of first-order NFEs. A set of necessary and sufficient conditions was presented that ensure the existence and uniqueness of a locally analytic solution to the aforementioned system of NFEs, and a series solution method that can be easily implemented via a MAPLE code was developed. Under these conditions, the convergence of the estimation error or the mismatch between the actual unmeasurable states and their estimates was analyzed and characterized in the presence of model uncertainty.

Finally, the last Chapter's methods could be generalized to include model inputs or time-varying process parameters, such as catalyst deactivation, enzymatic degradation, or other types of model uncertainty. This would further enlarge the range of applications of the proposed methods.

APPENDIX A

MAPLE Code for Chapter II Illustrative example

```
> restart:
> libname:="D:/archives/maple/nlp", libname:
> readlib(mtaylor):
> readlib(coeftayl):
> with( LinearAlgebra):
> with( linalg ):
> with ( NonlinearProgramming ):
> T:=0.000001:x10:=0:x20:=0:xa0:=10:xas:=2.697:xbs:=1.05:
fv:=28.423:k1:=50:k2:=100:k3:=10:
> Q:=x2^2+1E-5*(-p1*x1-p2*x2)^2:F1:=x1+((-x1*p1-  x2*p2)*
             (xa0-xas-x1)-(fv+k1+2*k3*xas)*x1-k3*x1^2)*T:
> F2:=x2+((x1*p1+x2*p2)*(xbs+x2)+k1*x1-(k2+fv)*x2)*T:
> N:=7:
> s:=mtaylor(V(x1,x2)-V(x10,x20)-D[1](V)(x10,x20)*x1-
D[2](V)(x10,x20)*x2,[x1=x10,x2=x20],N):
> sp:=subs([x1=F1,x2=F2],s):d:={}:q(1):={}:
```

```
> for j from 2 to N-1 do
    for i from 0 to j do
        p[i,j-i]:=(i!*(j-i)!)*coeftayl(s,[x1,x2]=
[x10,x20],[i,j-i]):
        q(j):=q(j-1) union {p[i,j-i]}:
        d:=d union q(j):
    od:
od:
> pde:=mtaylor(sp-s+Q,[x1=x10,x2=x20],N):c:={}:r(1):={}:
> for j from 2 to N-1 do
   for i from 0 to j do
      t[i,j-i]:=coeftayl(pde,[x1,x2]=[x10,x20],[i,j-i]):
      r(j):= r(j-1) union {t[i,j-i]}:
      c:=c union r(j):
    od:
od:
> fin:=solve(c,d):
> fin:
> sol:=subs(fin,s):
> obj:=subs([x1=-0.877307434,x2=-0.16], sol):
> fun:=algsubs(p2=x[2], algsubs(p1=x[1],obj)):
> infolevel['UnconstrainedNewton']:=2:
> infolevel['Optimize']:=2:
> infolevel['PrimalDualLogBarrier']:=2:
> numDecVars:=2:
> x_start:=<50,80>:
> UnconstrainedNewton( fun, numDecVars, x_start, 'convex','float[8]');
```

APPENDIX B

Existence and uniqueness conditions for the solution of the system of singular PDEs (3.6)

Under the following set of conditions, the system of first-order singular PDEs (3.6) admits a unique locally analytic and invertible solution $\bar{z} = T(\bar{x})$ in a neighborhood of the origin [60]:

Condition B.1. The Jacobian matrix $F = \frac{\partial \bar{f}}{\partial \bar{x}}(0)$ has eigenvalues $ki(i = 1, ..., n)$ with:

$$0 \notin co\{k_1, k_2, ..., k_n\} \tag{B.1}$$

where *co* stands for the convex hull of a set. Equivalently stated, the spectrum of F belongs to the Poincaré domain [3]. It should be pointed out, that this assumption has been recently relaxed in [69], where existence and uniqueness of a solution to the system of PDEs (3.6) is proved under the rather generic assumption that the spectrum of F lies wholly in the Siegel domain [3, 69].

Condition B.2.

The following matrix $\mathscr{O}$:

$$\mathscr{O} = \begin{bmatrix} C_0 \\ C_0F \\ \vdots \\ C_0F^{n-1} \end{bmatrix} \tag{B.2}$$

has rank n.

Condition B.3.

The following matrix $\mathscr{C}$:

$$\mathscr{C} = \begin{bmatrix} B & AB & \cdots A^{n-1}B \end{bmatrix} \tag{B.3}$$

has rank n. It can be shown that Conditions B.2 and B.3 are crucial in order to ensure local invertibility of the unknown solution $T(\bar{x})$ of (3.6) [60].

Condition B.4.

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

$$\sum_{i=1}^{n} m_i k_i = \lambda_i (j = 1, ..., n) \tag{B.4}$$

where all the m_i are non-negative integers that satisfy the condition:

$$\sum_{i=1}^{n} m_i > 0 \tag{B.5}$$

Conditions B.1 and B.4 are necessary for the existence and uniqueness of the unknown solution $T(\bar{x})$ of (3.6). In particular, Condition B.1 ensures the uniform convergence of the formal power series representation of the unique solution $T(\bar{x})$ that is guaranteed by Condition B.4, and hence, its analyticity property [60].

Let us now consider the problem of the development of a solution method for the system of PDEs (3.6). We would first like to point out, that the method of

characteristics for the system of first-order PDEs (3.6) can not be applied due to the singularity at the reference equilibrium point. However, as previously mentioned, the function $\bar{f}(\bar{x})$, as well as the solution $T(\bar{x})$ are locally analytic. Therefore, the proposed solution method is based on a multivariate Taylor series expansion of $\bar{f}(\bar{x})$, as well as the unknown solution $T(\bar{x})$, followed by a procedure that equates the Taylor coefficients of both sides of the system of PDEs (3.6). 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 $T(\bar{x})$, given the Taylor coefficients of $T(\bar{x})$ up to the order $N-1$ already calculated in previous recursive steps. It should be pointed out, that the above linear recursive formulas admit a compact mathematical representation if tensorial notation is used [60]. The linearity exhibited by the above recursive relations is precisely the mathematical reason, that allows the proposed series solution method for the system of singular PDEs (3.6) 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 (3.6) [61].

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