Global Observability and Detectability Analysis of Uncertain Reaction Systems and Observer Design

Jaime A. Moreno [a,1,2] and Denis Dochain [b,2,3]

[a] *Instituto de Ingeniería, UNAM, Automatización, Cd. Universitaria, C.P.04510 México D.F., MEXICO, JMorenoP@iingen.unam.mx, Fax: ++(52-55) 56 22 81 30*

[b] *CESAME, Université Catholique de Louvain, 4-6 avenue G. Lemaitre, 1348 Louvain-la-Neuve, Belgium. dochain@csam.ucl.ac.be*

Abstract

Observation issues is of fundamental importance for reaction systems due to the limited availability of on-line sensors and the uncertainties related in particular to the model dynamics. The objective of this work is to propose a methodology to make a global analysis of observability and detectability of such systems, with a particular concern about the design of unknown input observers.

Key words: Observability, indistinguishability, detectability, uncertain reaction systems, Unknown input observer

1 Introduction

Reaction systems is a class of nonlinear dynamical systems that is widely used in areas such as chemical and biochemical engineering, biomedical engineering, biotechnology, ecology, etc. (Robust) observation issues for this class of

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systems is of fundamental importance due to the limited availability of on-line sensors and the uncertainties related in particular to the model dynamics. It is not surprising that there is an intensive research activity to design observers, or software sensors, for these systems (Bastin and Dochain, 1990; Dochain and Vanrolleghem, 2001; Dochain, 2003). It is well known that the existence of observers for dynamical systems is intrinsically related to the observability or to the detectability of the system. However, there are few studies in the literature dealing with the observability, detectability properties of reaction systems. Most of these studies are local in nature (Dochain and Chen, 1992). However, a satisfactory solution to the observation problem is global since it seems unreasonable to require that the initial condition of the system is known up to a small error, when one of the motivations to use an observer is precisely the lack of information on this initial state!

The objective of this work is to propose a methodology to make a global analysis of observability and detectability of reaction systems. This is in contrast to the usual local results of the literature. When there are no uncertainties, the usual method to do a global observability analysis is by means of the observability map (Zeitz, 1989; Gauthier and Kupka, 2001). However, there is no systematic method to study detectability for nonlinear systems. In this work a methodology is presented to carry out a *global* observability/detectability analysis of *uncertain* reaction systems when the uncertainty is represented as an arbitrary and unknown input signal. No method is known to study observability for this kind of systems. The proposed method is an extension for the uncertain case of the idea used for the analysis of the induction machine under sensorless operation (Ibarra-Rojas *et al.*, 2004). Other approaches are given in (Ponzoni *et al.*, 2004), based on structural information, but restricted to non dynamical representations of the system in steady state. The cornerstone of this result is the *strongly indistinguishable trajectories* concept (internal trajectories of a system that are different under the same input/output behavior under uncertain inputs) and the main result is the *characterization* of *the complete set* of this kind of functions for the uncertain reaction system, including both types of indistinguishable trajectories: the divergent (non-observable) ones, i.e. those which are not possible to identify by input/output measurements, and the asymptotically convergent (detectable) ones, i.e. those that can be determined by the input/output behavior asymptotically. The proposed methodology achieves the desired characterization by constructing a nonlinear dynamical system, called *strongly indistinguishable dynamics*, whose set of solution trajectories corresponds to the aforementioned set of strongly indistinguishable behaviors, i.e. every solution trajectory of this system is an strongly indistinguishable trajectory for the studied system. Some sufficient conditions for an uncertain reaction system to be observable/detectable will be given.

When suitable detectability conditions are satisfied, then the construction of a (robust) observer is possible and a method to design them is given. Moreover, observability/detectability conditions are given, under which the convergence dynamics of the observers can be assigned. Since asymptotic observers (Bastin and Dochain, 1990; Dochain and Vanrolleghem, 2001; Dochain, 2003) are a special case of the proposed observers, our results justify the existence conditions of asymptotic observers by means of the detectability properties of the system. Finally the proposed results provide insights to analyse the conditions when the convergence dynamics of asymptotic observers can or cannot be assigned.

The paper is organised as follows. A general model of reaction systems is given in Section 2. Global observability/detectability properties are introduced for uncertain systems and their relationship with the existence of observers are studied in Section 3. The observability properties of uncertain reaction systems are analyzed in Sections 4 and 5, and their consequences for observer design are given in Section 6, where a method to design robust observers is given. Some examples in Section 7 illustrate the results of the paper.

2 Model of Reaction Systems

A general state-space model of reaction systems is generally obtained from mass and energy balances (Bastin and Dochain, 1990; Dochain *et al.*, 1992; Dochain and Vanrolleghem, 2001) :

$$\begin{aligned}\frac{dc}{dt} &= \bar{K}\varphi\left(c,T\right) + D\left(c_{in} - c\right) - Q_c\left(c,T\right) + \bar{F}\\ \frac{dT}{dt} &= -\frac{1}{\rho C_p}\Delta H^T\varphi\left(c,T\right) + D\left(T_{in} - T\right) - Q_T\end{aligned}$$

where $c \in \mathbb{R}^{n-1}$, $T \in \mathbb{R}$, $\bar{K} \in \mathbb{R}^{(n-1)\times q}$, $\varphi \in \mathbb{R}^q$, $D \in \mathbb{R}$, $Q_c \in \mathbb{R}^{n-1}$, $\bar{F} \in \mathbb{R}^{n-1}$, $\rho \in \mathbb{R}$, $C_p \in \mathbb{R}$, $\Delta H \in \mathbb{R}^q$, $Q_T \in \mathbb{R}$, $c_{in} \in \mathbb{R}^{n-1}$ and $T_{in} \in \mathbb{R}$ are the component concentration vector, the temperature, the stoichiometric coefficient matrix, the reaction rate vector, the dilution rate, the gaseous outflow rate vector, the feedrate vector, the density, the heat capacity, the reaction heat vector, the heat exchange term, and the inlet concentration vector and temperature, respectively. In most applications the measured variables are a subset of the state variables or, more generally, a linear combination of them.

This system can be written in a compact and generalized form as follows :

$$\Sigma_R : \begin{cases} \dot{x} = K\varphi\left(x\right) + D\left(x_{in} - x\right) - Q\left(x\right) + F \ , \\ y = Cx \ . \end{cases} \tag{1}$$

where $x \in \mathbb{R}^n$ is the state, and $y \in \mathbb{R}^m$ is the output vector. This model also includes the case when several reactors are considered, in which case $D \in \mathbb{R}^{n \times n}$ is a matrix. In practice the knowledge of the model is usually very uncertain, since the parameters and nonlinearities of the system are difficult to identify precisely; moreover they may change over time. In particular, the reaction rates are usually poorly known. This makes the observation problem challenging. In this paper we shall concentrate on the case when the reaction rates are unknown, but the rest of the model is assumed to be known, i.e. $u = F - Q(x) + Dx_{in}$ is considered a known signal (Bastin and Dochain, 1990). This uncertainty will be modelled as an (arbitrary) unknown input $w = \varphi(x)$.

3 Observability and Detectability concepts for nonlinear uncertain systems and existence of observers

Since the uncertainties in the reaction system (1) will be represented by unknown inputs, let us consider a general nonlinear system described by the following equations :

$$\Sigma : \begin{cases} \dot{x} = f(x, u, w) \ , \quad x(0) = x_0 \\ y = h(x) \ , \end{cases} \tag{2}$$

where $x \in \mathbb{R}^n$ is the state vector, $u \in \mathbb{R}^p$ is the input vector, $w \in \mathbb{R}^q$ is a vector of unknown inputs, $y \in \mathbb{R}^m$ is the output vector, and f and h are sufficiently smooth functions. The solution of (2) passing through x_0 at $t = 0$ and corresponding to the input function $u(\cdot)$ and $w(\cdot)$ is denoted as $x(t, x_0, u(\cdot), w(\cdot))$. In a similar way, let us denote the output $y(t, x_0, u(\cdot), w(\cdot)) = h(x(t, x_0, u(\cdot), w(\cdot)))$. Whenever there is no possible confusion, these will be simply denoted as $x(t)$ and $y(t)$. Let us assume in addition that the system Σ is *complete*, i.e. the state trajectories $x(t)$ are defined for every $t \geq 0$, every initial condition $x_0 \in \mathbb{R}^n$ and every input $u(\cdot) \in \mathcal{U}$, and $w(\cdot) \in \mathcal{W}$, where $\mathcal{U}$, $\mathcal{W}$ are classes of input functions.

A basic concept for systems without unknown inputs is that of indistinguishable states (Hermann and Krener, 1977). Roughly speaking, two states are said to be indistinguishable if they are different although both the input and the output of the system are identical. The importance of this definition comes from the fact that observer's existence for the system strongly relies on the existence (and the type) of this kind of functions. For systems with unknown inputs (2), similar concepts can be introduced.

Definition 1 ***(Strong Indistinguishability and Observability,*** **and** ***Strong(*) Detectability).*** *Consider for system (2) an input $u(\cdot)$, an initial condition $x \in \mathbb{R}^n$ and an unknown input $w(\cdot)$. If $\bar{x} \in \mathbb{R}^n$, $\bar{x} \neq x$, is such that*

$y(t,x,u(\cdot),0) = y(t,\bar{x},u(\cdot),w(\cdot))$, $\forall t \in [0,\infty)$ and for some $w(\cdot) \in \mathcal{W}$, then $\bar{x}$ is a strongly $u(\cdot)$-indistinguishable *state of x. $\mathcal{I}^{UI}_{(u,x)}$ denotes the set of strongly $u(\cdot)$-indistin-guishable states of x.*
System (2) is strongly observable *if for every $x \in \mathbb{R}^n$ and every $u(\cdot) \in \mathcal{U}$, $\mathcal{I}^{UI}_{(u,x)} = \{x\}$.*
System (2) is strongly detectable *if for every $x \in \mathbb{R}^n$, every $u(\cdot) \in \mathcal{U}$ and for every $\bar{x} \in \mathcal{I}^{UI}_{(u,x)}$ and the corresponding $w(\cdot)$ that renders $\bar{x}$ indistinguishable* $\lim_{t\to\infty} \|x(t,\bar{x},u(t),w(\cdot)) - x(t,x,u(t),0)\| = 0$.

System (2) is strong* detectable *if for some $x,\bar{x} \in \mathbb{R}^n$, $u(\cdot) \in \mathcal{U}$ and $w(\cdot) \in \mathcal{W}$ it happens that* $\lim_{t\to\infty} \|y(t,\bar{x},u(t),w(t)) - y(t,x,u(t),0)\| = 0$ *, then it follows that* $\lim_{t\to\infty} \|x(t,\bar{x},u(t),w(t)) - x(t,x,u(t),0)\| = 0$.

Note that strong detectability excludes the existence of diverging strongly indistinguishable trajectories.

It may be surprising that two detectability definitions have been introduced. For LTI systems without unknown inputs it is well-known that if the unobservable subsystem is asymptotically stable then if as $t \to \infty$ $y(t) \to 0$ then $x(t) \to 0$. However, for continuous time systems with unknown inputs this is not longer the case, as has been pointed out by (Hautus, 1983).

Remark 2 *It is clear that strong* detectability implies strong detectability, but the converse is not true. Moreover, strong observability implies strong detectability, but it does not necessarily imply strong* detectability.*

These properties are indeed related to the existence of Unknown Input Observers (UIO).

Definition 3 ***(UI Observer)*** *Consider a system*

$$\Omega : \begin{cases} \dot{z} = \varphi(z,u,y) \ , & z(0) = z_0 \\ \hat{x} = \chi(z,u,y) \ , & \end{cases} \tag{3}$$

where $z \in \mathbb{R}^r$ is the state vector and φ, χ are functions defined in $(z,u,y) \in \mathbb{R}^r \times \mathbb{R}^p \times \mathbb{R}^m$. $z(t,z_0,u,y)$ denotes a solution of (3) passing through z_0 at $t = 0$ and corresponding to (u,y).
System (3) is called an unknown input observer (UIO) *for system (2) if $\exists z_0 \in \mathbb{R}^r$ such that $\forall x_0 \in \mathbb{R}^n$, $\forall u(\cdot) \in \mathcal{U}$ and $\forall w(\cdot) \in \mathcal{W}$*

$$\lim_{t\to\infty} \|\hat{x}(t,z_0,u,y(t,x_0,u,w)) - x(t,x_0,u,w)\| = 0 \ .$$

Note that in this definition no major restriction has been imposed on the observer, except for the convergence of the observer for *every* trajectory, i.e.

initial condition and input, of the system.

For LTI systems it is shown by (Hautus, 1983) that strong* detectability is equivalent to the existence of an UIO and that strong detectability or observability are not sufficient for the existence of an UIO. Let us now partially generalize the concept for nonlinear systems.

The following result is indeed valid for every reasonable definition of observer, since it depends on a structural restriction of the system and not on the structure of the observer.

Lemma 4 *If system (2) has an unknown input global observer, then it is strong* detectable. Moreover, if the convergence of the observer can be assigned arbitrarily fast, then it is strongly observable.*

PROOF. Suppose that system (2) is not strong* detectable. Then there exist an input $u(\cdot)$, two states $x_1, x_2 \in \mathbb{R}^n$ and an unknown input $w(\cdot)$ such that as $t \to \infty$, $y(t, x_1, u, 0) \to y(t, x_2, u, w)$, but $x(t, x_1, u, 0) - x(t, x_2, u, w) \nrightarrow 0$. For an UI (global) observer Ω of Σ, there exists $z_0 \in \mathbb{R}^r$ such that $\hat{x}(t, z_0, u, y(t, x_1, u, 0)) \to x(t, x_1, u, 0)$ and $\hat{x}(t, z_0, u, y(t, x_2, u, w)) \to x(t, x_2, u, w)$. Note $\hat{x}(t, z_0, u, y(t, x_1, u, 0)) \to \hat{x}(t, z_0, u, y(t, x_2, u, w))$. But since

$$\begin{aligned}\lim_{t\to\infty} \{x(t, x_1, u, 0) - x(t, x_2, u, w)\} = \\ = \lim_{t\to\infty} \{x(t, x_1, u, 0) - \hat{x}(t, z_0, u, y_1)\} + \\ + \lim_{t\to\infty} \{x(t, x_2, u, w) - \hat{x}(t, z_0, u, y_2)\} = 0 \ ,\end{aligned}$$

the assumption on x_1, x_2 is contradicted.
To prove the second assertion, suppose by contradiction that there are two convergent indistinguishable trajectories. Then an observer cannot converge to the correct state at a rate greater than the convergence rate of the trajectories. □

From this lemma it is clear that for studying the possibility of estimating state trajectories of a given dynamical system, one can first investigate the existence of robustly indistinguishable trajectories and then determine if they are converging or not, i.e. if the system is robustly detectable or observable.

4 The error and indistinguishable dynamics of reaction systems

The conditions given above are abstract and not checkable. The objective of this section is to introduce a dynamical interpretation of the concepts introduced previously that will be used in the following section to derive necessary conditions for the existence of global observers. This dynamic characterization, although possible for a general nonlinear system, will be derived here for the case of interest in the paper, the uncertain reaction system (1). It will be assumed that the model is well-known, except for the reaction rates that are completely unknown, so that they can be considered as unknown inputs. This is a very strong assumption but it leads to simple and useful results.

The following Gedanken-experiment leads to the desired characterization of strong* and strong detectability: two identical systems (1) but with different initial conditions and reaction rates, i.e. unknown inputs $\varphi(x) = w$, evolve in time

$$\begin{aligned} \dot{x}_i &= Kw_i - Dx_i + u \ , \ x_i(0) = x_{i0} \ , \\ y_i &= Cx_i \ , \qquad i = 1, 2 \ . \end{aligned}$$

Introducing the variables $x = x_1$, $y = y_1$, $w = w_1$ and $\tilde{x} = x_1 - x_2$, $\tilde{y} = y_1 - y_2$, $\tilde{w} = w_1 - w_2$, the error dynamics of the plant are given by

$$\begin{aligned} \dot{x} &= Kw - Dx + u \ , \ x(0) = x_0 \ , \\ \dot{\tilde{x}} &= K\tilde{w} - D\tilde{x} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ y &= Cx \ , \\ \tilde{y} &= C\tilde{x} \ . \end{aligned} \tag{4}$$

Since for this system the evolution of x does not affect the error state $\tilde{x}$, the basic properties can be studied via the reduced linear system

$$\begin{aligned} \dot{\tilde{x}} &= -D\tilde{x} + K\tilde{w} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ \tilde{y} &= C\tilde{x} \ . \end{aligned} \tag{5}$$

Consider also the linear Differential-Algebraic (DA) system,

$$\begin{aligned} \dot{\tilde{x}} &= -D\tilde{x} + K\tilde{w} \ , \ \tilde{x}(0) = \tilde{x}_0 \ , \\ 0 &= C\tilde{x} \ . \end{aligned} \tag{6}$$

derived from (5) by setting $\tilde{y}(t) = 0$ for all $t \geq 0$. This system will be called the (reduced) *Strongly Indistinguishable Dynamics* of the plant (1) with unknown reaction rates. Strong(*) detectability and observability of the plant can be determined and characterized analyzing the properties of the solution set of the Strong Indistinguishable Dynamics. The following result is a simple consequence of the definitions.

Lemma 5 *Consider the system (1), with unknown reaction rates.*

(1) Two trajectories are strongly indistinguishable *if and only if they are of the form* $x(t, x_0, u(t), w(\cdot))$ *and* $x(t, x_0, u(t), w(\cdot)) + \tilde{x}(t, \tilde{x}_0, \tilde{w}(\cdot))$ *, where* $x(t)$ *is a solution of (1) and* $\tilde{x}(t)$ *is a solution of (6).*
(2) The system is strongly detectable *if and only if the constrained system (6) is globally asymptotically stable.*
(3) The system is strongly observable *if and only if the constrained system (6) is trivial, i.e. the only solution is* $\tilde{x}(t) = 0$*.*
(4) The system is strong* detectable *if and only if for the system (5) whenever* $\lim_{t\to\infty} \tilde{y}(t) = 0$ *it follows that* $\lim_{t\to\infty} \tilde{x}(t) = 0$*.*

In the special case considered in this paper, the indistinguishable dynamics (5) is very simple, since it is decoupled from the plant and because it is a linear time-varying system. This allows a very deep analysis that is seldom possible.

Recall that a usual characterization of the zeros (or zero dynamics) of a system corresponds to the set of pairs of initial conditions and inputs, such that the output of the system is zero for all the time. This means that the *zero dynamics* of the indistinguishable dynamics (5) is given by the constrained system (6). Note that the strong indistinguishable trajectories correspond to the trajectories of the zero dynamics, that strong observability is equivalent to the absence of strong indistinguishable trajectories, i.e to the absence of zeros and strong detectability coincides with the asymptotic stability of the zero dynamics.

Lemma 5 gives a dynamical interpretation of the observability/detectability concepts for the specific case considered. It is clear that this idea can be used for more general systems although the obtained indistinguishability dynamics systems are, in general, not so simple as here. Compared to the usual observability criteria that are based on the construction of the observability map with the vector fields, this characterization has several advantages : 1) The approach is not local whether in time nor in the state space. 2) It allows to determine detectability, what is usually impossible in the other criteria. 3) The dynamical interpretation is appealing. 4) Several nonlinear tools can be used to make the analysis, as for example the characterization of the zero dynamics in geometric control. 5) Lyapunov functions can be used for the characterization of the properties. 6) It is of very general nature. No special smoothness or structural properties are necessary. 7) For systems with unknown inputs there is no observability test based on the system vector fields in the literature.

5 Detectability analysis for uncertain reaction systems

The analysis of the error dynamics (4) provides basic information for the design of UIO's. Since strong* detectability is a necessary condition for the existence of UIO (see Lemma 4), the objective is to determine conditions on the system, such that when $\tilde{y} \to 0$ as $t \to \infty$, it follows that $\tilde{x} \to 0$ as $t \to \infty$. Since D is in general a time varying matrix the results for the LTI case of (Hautus, 1983) do not apply. It is clear that asymptotic stability of the zero dynamics (6), i.e. *asymptotic minimum phaseness*, or equivalently strongly detectability, is a necessary property. Sufficient conditions (in the LTI case also necessary) are:

Proposition 6 *Consider the system (5) with constant matrices C and K and a uniformly bounded time-varying matrix D. $\tilde{y} \to 0$ as $t \to \infty$ implies $\tilde{x} \to 0$ as $t \to \infty$ if*

(1) $\operatorname{rank}(CK) = \operatorname{rank}(K)$,
(2) System (5) is exponentially minimum phase, i.e. the system described by the DAE (6) has an exponentially stable equilibrium point.

PROOF. Define a regular output transformation

$$\bar{y} = \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = S\tilde{y} = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} \tilde{y} \tag{7}$$

where $S_1 \in \mathbb{R}^{q \times m}$, $S_2 \in \mathbb{R}^{(m-q) \times m}$ and S is regular. Due to condition (1) S_1, S_2 and M, such that $MK = 0$, can be so selected, that

$$T = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} = \begin{bmatrix} S_1 C \\ S_2 C \\ M \end{bmatrix},$$

defines a state transformation $z = T\tilde{x}$. Defining $z_i \triangleq T_i \tilde{x}$, $i = 1, 2, 3$, system (5) in the new coordinates is given by

$$\begin{aligned} \dot{z}_1 &= \bar{D}_{11} z_1 + \bar{D}_{12} z_2 + \bar{D}_{13} z_3 + w \\ \dot{z}_2 &= \bar{D}_{21} z_1 + \bar{D}_{22} z_2 + \bar{D}_{23} z_3 \\ \dot{z}_3 &= \bar{D}_{31} z_1 + \bar{D}_{32} z_2 + \bar{D}_{33} z_3 \\ \bar{y} &= \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = \bar{C} z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \end{aligned} \tag{8}$$

where

$$\bar{D} = -TDT^{-1} = \begin{bmatrix} \bar{D}_{11} & \bar{D}_{12} & \bar{D}_{13} \\ \bar{D}_{21} & \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{31} & \bar{D}_{32} & \bar{D}_{33} \end{bmatrix},$$
$$\bar{C} = SCT^{-1} = \begin{bmatrix} I_q & 0 & 0 \\ 0 & I_{m-q} & 0 \end{bmatrix}.$$

The zero dynamics of the original system in the new coordinates is then

$$\dot{z}_3 = \bar{D}_{33} z_3 \ , \ 0 = \bar{D}_{13} z_3 + w \ , \ 0 = \bar{D}_{23} z_3 \tag{9}$$

that by hypothesis is assumed to be exponentially stable. By standard results of input/output stability of LTV systems (Callier and Desoer, 1991), it follows that when $z_1 \to 0$ and $z_2 \to 0$ then $z_3 \to 0$ as $t \to \infty$ in system (8) and therefore $\tilde{y} \to 0$ implies $\tilde{x} \to 0$ for (5). □

Remark 7 *Note that the first condition implies that $m \geq q$, i.e. the number of measurements has to be larger than the number of unknown inputs.*

Remark 8 *Exponential minimum phaseness has to be required, since for LTV systems asymptotic stability does not guarantee input/output stability (see (Rugh, 1993)) that is required in the subsystem z_3 in (8). To clarify this observation consider the scalar system with bounded coefficients*

$$\dot{x}(t) = \frac{-2t}{t^2+1} x(t) + u(t) \ , \ x(t_0) = x_0 \ ,$$
$$y(t) = x(t) \ .$$

This system is not exponentially stable since the transition matrix is given by

$$\Phi(t, t_0) = \frac{t_0^2 + 1}{t^2 + 1} \ .$$

But it is uniformly stable and the zero-input response goes to zero for every initial state. However, it is not BIBO stable and a vanishing input does not produce a vanishing output, i.e. $u \to 0 \not\Rightarrow y \to 0$ as $t \to \infty$. To see this consider the output response for $t_0 = 0$ and $x_0 = 0$

$$y(t) = \frac{1}{t^2+1} \int_0^t \left(\tau^2 + 1\right) u(\tau)\, d\tau \ .$$

For $u = 1$ the output $y(t) = (t^3/3 + t) / (t^2 + 1)$ is unbounded. For $u(t) = t^r / (t^2 + 1)$, with $1 < r < 2$, $u(t) \to 0$ but $y(t) = t^{(r+1)} / (r+1)(t^2+1)$ is unbounded! And so in general exponential stability has to be imposed. However, exponential minimum phaseness is also not necessary. Consider for example *subsystem z_3 in (8) and that $\bar{D}_{31} = 0$ and $\bar{D}_{32} = 0$. In this case asymptotic minimum phaseness is sufficient to guarantee the convergence.*

Remark 9 *It is interesting to note that it is possible to have a system that is strong* detectable and strongly observable. This is the case when the only solution of (9) is $z_3 = 0$. However, this is not possible if $m = q$.*

6 Observer Design

For LTI systems the conditions in the previous proposition are also sufficient for the existence of an UIO. For time-varying systems this seems not to be the case. However, under some mild further assumptions (always satisfied in the LTI case), an UIO can be constructed. For simplicity it will be assumed that the plant has been transformed according to the state and output transformation introduced in the proof of Proposition 6.

In the following result two observability concepts related to a linear time varying system

$$\dot{x}(t) = A(t)\,x(t)\ ,\ y(t) = C(t)\,x(t)\ , \tag{10}$$

with bounded matrices, will be required. System (10) is said to be *Uniformly Completly Observable* (UCO) (Anderson and Moore, 1990) if there exist some $T > 0$ and some $\alpha > 0$ such that for every $t \geq 0$ the observability Grammian satisfies $O(t, t+T) = \int_t^{t+T} \Phi^T(t+T,\tau)\,C^T(\tau)\,C(\tau)\,\Phi(t+T,\tau)\,d\tau > \alpha I$, where $\Phi(t, t_0)$ is the transition matrix of the system. An UCO system has the property that there exists a bounded matrix $L(t)$ such that

$$\dot{x}(t) = [A(t) + L(t)\,C(t)]\,x(t)\ , \tag{11}$$

has arbitrary degree of stability, that is, given $\beta > 0$, one can find $L(t)$ such that $e^{\beta t}x(t) \rightarrow 0$ for all $x(t_0)$. In the same spirit of this definition it will be said that system (10) is *uniformly detectable* if there exists a bounded matrix $L(t)$ such that system (11) is uniformly asymptotically stable, i.e. there exists some $\gamma > 0$ such that $e^{\gamma t}x(t) \rightarrow 0$ for all $x(t_0)$. Note that in this case it is not necessarily possible to achieve an arbitrary degree of stability.

Proposition 10 *Consider the reactor system (1) with constant matrices C and K, and a uniformly bounded time-varying matrix D, that satisfies the* *conditions of Proposition 6 and is represented in new coordinates as follows :*

$$\begin{aligned}
\dot{\xi}_1 &= \bar{D}_{11}\xi_1 + \bar{D}_{12}\xi_2 + \bar{D}_{13}\xi_3 + w + u_1 \\
\dot{\xi}_2 &= \bar{D}_{21}\xi_1 + \bar{D}_{22}\xi_2 + \bar{D}_{23}\xi_3 + u_2 \\
\dot{\xi}_3 &= \bar{D}_{31}\xi_1 + \bar{D}_{32}\xi_2 + \bar{D}_{33}\xi_3 + u_3 \\
\bar{y} &= \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \end{bmatrix} = \bar{C}\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} .
\end{aligned} \tag{12}$$

Consider the subsystem independent of the unknown input

$$\begin{aligned}
\dot{\xi}_2 &= \bar{D}_{21}\xi_1 + \bar{D}_{22}\xi_2 + \bar{D}_{23}\xi_3 + u_2 \\
\dot{\xi}_3 &= \bar{D}_{31}\xi_1 + \bar{D}_{32}\xi_2 + \bar{D}_{33}\xi_3 + u_3 \\
\bar{y}_2 &= [0, I, 0]\,\xi = \xi_2 \ ,
\end{aligned} \tag{13}$$

and a reduced order UIO for the plant of the form

$$\begin{aligned}
\dot{\hat{\xi}}_2 &= \bar{D}_{21}\bar{y}_1 + \bar{D}_{22}\hat{\xi}_2 + \bar{D}_{23}\hat{\xi}_3 + u_2 + L_1\left(\hat{y}_2 - y_2\right) \\
\dot{\hat{\xi}}_3 &= \bar{D}_{31}\bar{y}_1 + \bar{D}_{32}\hat{\xi}_2 + \bar{D}_{33}\hat{\xi}_3 + u_3 + L_2\left(\hat{y}_2 - y_2\right) \\
\hat{y}_2 &= [I, 0]\,\hat{\xi} = \hat{\xi}_2 \ ,
\end{aligned} \tag{14}$$

(1) If the pair $\left([I,0], \begin{bmatrix} \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{32} & \bar{D}_{33} \end{bmatrix}\right)$ *is UCO, then (14) is a reduced order UI observer whose convergence dynamics can be arbitrarily assigned.*

(2) If the pair $\left([I,0], \begin{bmatrix} \bar{D}_{22} & \bar{D}_{23} \\ \bar{D}_{32} & \bar{D}_{33} \end{bmatrix}\right)$ *is uniformly detectable, then (14) is a reduced order UI observer.*

PROOF. The dynamics of the estimation error between the observer (14) and the subsystem (13) is

$$\dot{e} = \left(\begin{bmatrix} \bar{D}_{22} + L_1 & \bar{D}_{23} \\ \bar{D}_{32} + L_2 & \bar{D}_{33} \end{bmatrix}\right) e \ , \ e = \begin{bmatrix} \hat{\xi}_2 - \xi_2 \\ \hat{\xi}_3 - \xi_3 \end{bmatrix} .$$

If condition (2) is satisfied then L exists such that $e \to 0$ uniformly. If moreover, condition (1) is satisfied, then any desired degree of stability can be reached. □

It is interesting to note that the results derived in the literature under the name asymptotic observer (Bastin and Dochain, 1990), that are able to estimate the state of a bioreactor without knowledge of the reaction rates, are special cases of the results in this paper. In fact, our results are a justification from the observability/detectability point of view of the asymptotic observers.

Note that if Condition (1) of the Proposition 10 is satisfied, then the system has to be strongly observable, whereas Condition (2) implies strong* detectability. If in model (12), there is no measurement $\bar{y}_2$, then the state ξ_2 does not exist and Condition (1) of the Proposition 10 cannot be satisfied, while Condition (2) corresponds to the exponential stability of the system $\dot{x} = \bar{D}_{33}x$.

In particular if D is a scalar, i.e. $D = d\mathbb{I}$, then if the measurements are selected such that condition (1) of Proposition 6 is satisfied, then condition (2) is equivalent to the persistency of excitation of the input $d\,(t)$ (Bastin and Dochain, 1990). In this case it is however impossible to satisfy condition (1) of Proposition 10, and therefore it is not possible to assign the convergence dynamics of the UIO, no matter how the measurements are selected.

7 Examples

Some examples illustrate the use and advantages of the proposed method.

7.1 Single-tank process

Consider the following reaction scheme of an oxidation process with a parallel path

$$\begin{aligned} A + C &\longrightarrow B \\ B + C &\longrightarrow D \ . \\ A + C &\longrightarrow D \end{aligned}$$

If A and C are the external reactancts and C_A, C_B and C_C are measured, the dynamics of the system in a CSTR is given by the equation (1), i.e.

$$\begin{aligned} \dot{x} &= K\varphi\,(x) - Dx + u \ , \\ y &= Cx \ . \end{aligned}$$

with

$$K = \begin{bmatrix} -1 & 0 & -1 \\ 1 & -1 & 0 \\ -1 & -1 & -1 \\ 0 & 1 & 1 \end{bmatrix}, \quad x = \begin{bmatrix} C_A \\ C_B \\ C_C \\ C_D \end{bmatrix}, \quad \varphi(x) = \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \end{bmatrix}$$

$$u = \begin{bmatrix} F_A \\ 0 \\ F_C \\ 0 \end{bmatrix}, \quad C = \begin{bmatrix} 1\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,1\,0 \end{bmatrix},$$

and D is scalar. The system is strong* detectable if both conditions of Proposition 6 are satisfied. Condition (1) is easily seen to be fulfilled, since $\operatorname{rank}(CK) = \operatorname{rank}(K) = 3$. To check condition (2) the system is brought to the form (8) through the state transformation $z_1 = \begin{bmatrix} \tilde{x}_1 \; \tilde{x}_2 \; \tilde{x}_3 \end{bmatrix}^T$, $z_3 = \tilde{x}_4 + \tilde{x}_1 + \tilde{x}_2$

$$\begin{aligned} \dot{z}_1 &= CKw - Dz_1 \\ \dot{z}_3 &= -Dz_3 \ . \end{aligned}$$

System (6) corresponds then to the scalar equation $\dot{z}_3 = -Dz_3$, that is exponentially stable if $D(t)$ is a persistently exciting signal, i.e. if there exist $\alpha, T > 0$ such that for all $t \geq 0$ it is satisfied that $\int_t^{t+T} D(\tau)\, d\tau \geq \alpha$. In this case condition (2) of Proposition 6 is also satisfied.

Since then condition (2) of Proposition 10 is satisfied the system

$$\dot{\zeta} = -D\zeta - F_A$$

is a reduced order UI observer (or an asymptotic observer) for the plant, and $\zeta \to x_1 + x_2 + x_4$ exponentially fast, when $D(t)$ is a persistently exciting signal. Note that the convergence velocity cannot be assigned.

7.2 Multi-tank process

Consider an activated sludge process with an aeration tank, where a single reaction $S \to X$ occurs, and a (perfect) sedimentation tank, with no reaction since only the biomass X_R is recycled. If V and V_s are the volumes of each tank, q_{in} is the inlet flow rate, R and W are the recycle and wastage ratios, the dynamics is given by the equations (1), i.e.

$$\dot{x} = K\varphi(x) - Dx + u \ ,$$
$$y = Cx \ .$$

with

$$K = \begin{bmatrix} -k \\ 1 \\ 0 \end{bmatrix} \ , \ x = \begin{bmatrix} S \\ X \\ X_R \end{bmatrix} \ , \ u = \begin{bmatrix} F_S \\ 0 \\ 0 \end{bmatrix} \ ,$$

$$\varphi(x) = \mu(S)\,X \ , \ D = q_{in} \begin{bmatrix} \frac{1+R}{V} & 0 & 0 \\ 0 & \frac{1+R}{V} & -\frac{R}{V} \\ 0 & -\frac{W+R}{V_s} & \frac{1+R}{V_s} \end{bmatrix} \ .$$

Consider two measurement cases.

Case 1: If only the substrate S is measured, i.e. $C = \begin{bmatrix} 1 \ 0 \ 0 \end{bmatrix}$. The system is strong* detectable if both conditions of Proposition 6 are satisfied. Condition (1) is easily seen to be fulfilled. To check condition (2) the system is brought to the form (8) through the state transformation $z_1 = \tilde{x}_1$, $z_3 = \begin{bmatrix} \tilde{x}_1 + k\tilde{x}_2 \ \tilde{x}_3 \end{bmatrix}^T$

$$\dot{z}_1 = -kw - q_{in}\frac{1+R}{V}z_1$$
$$\dot{z}_3 = -q_{in}Bz_1 + q_{in}Az_3 \ ,$$

where

$$A = \begin{bmatrix} -\frac{1+R}{V} & k\frac{R}{V} \\ \frac{W+R}{kV_s} & -\frac{1+R}{V_s} \end{bmatrix} \ , \ B = \begin{bmatrix} 0 \\ \frac{W+R}{kV_s} \end{bmatrix} \ .$$

System (6) corresponds then to the dynamics

$$\dot{z}_3 = q_{in}Az_3 \ .$$

Matrix A is Hurwitz, since its characteristic polynomial is $p(s) = s^2 + \frac{(1+R)(V+V_s)}{VV_s}s + \frac{1+(2-W)R}{VV_s}$ and $0 \leq W \leq 1$. If $\lim_{t\to\infty}\int_{t_0}^{t} q_{in}(\tau)\,d\tau = \infty$ then this last system is asymptotically stable, and it is exponentially stable if $q_{in}(t)$ is a persistently exciting signal, i.e. if there exist $\alpha, T > 0$ such that for all $t \geq 0$ it is satisfied that $\int_t^{t+T} q_{in}(\tau)\,d\tau \geq \alpha$. In the last case condition (2) of Proposition 6 is also satisfied.

In the last case the condition (2) of Proposition 10 is satisfied and the system

$$\dot{\zeta} = -q_{in}BS + q_{in}A\zeta + \begin{bmatrix} F_S \\ 0 \end{bmatrix}$$

is a reduced order UI observer (or an asymptotic observer) for the plant, and $\zeta \to \begin{bmatrix} S + kX \\ X_R \end{bmatrix}$ exponentially fast, when $q_{in}(t)$ is a persistently exciting signal. However the convergence velocity cannot be assigned.

Case 2: If both substrate S and biomass X concentrations are measured, i.e. $C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$, it is clear from the previous analysis that the system is strong* detectable. Moreover, if for some $t \geq 0$, $q_{in}(t) \neq 0$, then the system is strongly observable. If $q_{in}(t)$ is a persistently exciting signal then condition (1) of Proposition 10 is satisfied and the system

$$\dot{\zeta} = -q_{in}BS + q_{in}A\zeta + \begin{bmatrix} F_S \\ 0 \end{bmatrix} + \gamma (S + kX - \hat{y})$$

$$\hat{y} = \begin{bmatrix} 1 & 0 \end{bmatrix} \zeta$$

is an UI observer for the plant, and $\zeta \to \begin{bmatrix} S + kX \\ X_R \end{bmatrix}$ exponentially fast, when $q_{in}(t)$ is a persistently exciting signal and the output injection gain γ is adequately designed. Moreover, the convergence velocity can be assigned arbitrarily. Indeed note that the estimation error dynamics is given by

$$\dot{\varepsilon} = q_{in} \left(A + L \begin{bmatrix} 1 & 0 \end{bmatrix} \right) \varepsilon \ ,$$

when the observer gain is selected as $\gamma = q_{in}L$. Since the eigenvalues of the matrix $\left(A + L \begin{bmatrix} 1 & 0 \end{bmatrix} \right)$ can be assigned arbitrarily, the exponential convergence of ε to zero can be assigned arbitrarily fast as long as $q_{in}(t)$ is a persistently exciting signal.

8 Concluding remarks

In this paper a new method has been proposed for the characterization of the observability/detectability properties of uncertain reaction systems, when the uncertainty is modeled as an arbitrary unknown input. A fairly complete characterization of these properties for the reactor system with unknown reaction rates has been obtained using this method and sufficient conditions for the possibility of constructing robust (asymptotic) observers have been given. These initial results open the possibility to study further other situations in a methodological manner. This will be pursued in future work.

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