Unknown Inputs and Reaction Rates Estimation in a CSTR with Full Concentration Vector Measurement

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Abstract: We address the problem of estimating the instantaneous reaction rates of the mass conversion taking place in an isothermal and isobaric continuous stirred tank reactor, CSTR, subject to a constant dilution rate. In addition to the estimation of the reaction rates, we also obtain an estimate of the influxes to the reactor. Our methodology requires the knowledge of the stoichiometric matrix and all the concentrations online, as well as the dilution rate. The observer is based on a generalised version of the Super-Twisting Algorithm, STA, which allows us to estimate in finite-time the unmeasured variables. The applicability of the observer is shown by a numerical simulation.

Keywords: Observers; reaction rate estimation; bioprocess; discontinuous observers; sliding modes.

1. INTRODUCTION

Population dynamics show how the number of a particular species change over time due to their birth and death of individuals along with their interaction with another species. When the number of individuals is large, one may consider an ordinary differential equation to represent its mathematical model. Such a mathematical model is in general nonlinear and comprise the stoichiometric coefficients, kinetic parameters, reaction networks, and influxes and effluxes of a control volume.

When considering a (bio)chemical process, a common reactor is a batch reactor in which the reactant species are initially added in order to allow them for the products to be formed. Once finished, the content of the reactor is extracted to obtain the products of the reaction. When a continuous process is preferred, both an influx and efflux to the reactor may be considered. The influx has fresh media with substrates to be converted into products and the content of the reactor is constantly extracted to obtain the products. When the volumetric rate of the influx and efflux is the same, they can be characterised by the dilution rate. In the following we consider such continuous reactor and denote it as continuous stirred-tank reactor, CSTR.

In general, it is difficult to model a biochemical process since the reaction rates that compose its mathematical model are unknown given that key processes in the network are abstracted in a single reaction and thus it is not a simple interaction of two species. However several reaction rates have been used to model particular interaction in bioprocesses as Monod, Haldane, Contois, Hill kinetics, among others. We refer the interested reader to (Bastin and Dochain, 2013), for a study of modelling, control, and estimation in reaction networks.

The reaction rates, however, are needed to monitor and control the process or for the design of the reactor itself. Hence it is important to know the instantaneous value of the reaction rate, especially if the functional form of the reaction rate is not known. In (Farza et al. (1998); Mhamdi and Marquardt (2004); Nuñez et al. (2013); Vargas et al. (2014); Reza López et al. (2023)) the authors design an observer of reaction rates for a class of nonlinear systems. In turn, works like (Dochain et al. (1992); López-Caamal and Moreno (2016); Czyżniewski and Łangowski (2024)) design observers for both the unmeasured states and reaction rates.

The Super-Twisting Algorithm, STA, is a second order sliding mode that steers its state and its derivative to zero exponentially (Levant, 1993). In works like (Moreno and Osorio, 2012) the finite-time stability was shown via a Lyapunov stability analysis and in (Moreno, 2012) the Lyapunov stability of more general second order algorithms are analysed. In turn, multivariable versions of the STA may be found in (Nagesh and Edwards (2014); López-Caamal and Moreno (2019)), among others.

This paper presents an observer of unknown concentrations in the influx along with the reaction rates of the network. We require that the number of species in the influx plus the number of the reaction rates equal that of the species in the network. Furthermore, we consider an online measurement of all the species in the network. Our observer has a correction term that endows the observation error with the dynamics of the Multivariable Unitary

Super-Twisting Algorithm. MUSTA, described in (López-Caamal and Moreno, 2015; López-Caamal and Moreno, 2019). Thus, the observation error dynamics is finite-time stable and all the estimates converge at the same time. In addition, such observer is robust to a matched, constant perturbation. In the scope of the current paper, such a perturbation is the derivative of the reaction rates and influxes, as discussed in §2.

Along the document, we use $\overline{\lambda}(\circ)$ (resp. $\underline{\lambda}(\circ)$) to denote the largest (smallest, resp.) eigenvalue of the argument. In turn $\otimes$ denotes the matrix Kronecker product.

2. MODEL DESCRIPTION

The mathematical model of a CSTR is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}(t) = \mathbf{N}\mathbf{v}(\mathbf{c}(t)) - \mathbf{q}\left(\mathbf{c}(t)\right) + d\left(\mathbf{B}\mathbf{f}(t) - \mathbf{c}(t)\right), \tag{1}$$

where

$$\mathbf{c} : \mathbb{R} \to \mathbb{R}^n \text{ is the concentration vector;} \tag{2a}$$
$$\mathbf{v} : \mathbb{R}^n \to \mathbb{R}^m \text{ is the reaction rate vector;} \tag{2b}$$
$$\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^n \text{ is the gasification vector;} \tag{2c}$$
$$\mathbf{f} : \mathbb{R} \to \mathbb{R}^r \text{ is the influx concentration vector;} \tag{2d}$$
$$\mathbf{N} \in \mathbb{R}^{n\times m} \text{ is the stoichiometric matrix;} \tag{2e}$$
$$\mathbf{B} \in \mathbb{R}^{n\times r} \text{ is the input matrix; and} \tag{2f}$$
$$d \in \mathbb{R}_+ \text{ is the dilution rate.} \tag{2g}$$

Assumption 1. We assume as known (i) the concentration vector, (ii) the gasification rate, (iii) the stoichiometric matrix (iv) the input matrix, and (v) the dilution rate, which we consider to be constant and different from zero.

In general it is not possible to have an online measurement of the full concentration vector; here, however, we solely focus on the estimation of the unknown input, $\mathbf{f}(t)$, and the reaction rate vector, $\mathbf{v}(\mathbf{c})$; and leave the concentrations estimation for future work.

In this light, we may restate (1) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}(t) = -\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}(t)\right)\right) + \mathbf{M}\mathbf{z}(t) \tag{3a}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z}(t) = \boldsymbol{\eta}(t), \tag{3b}$$

where

$$\mathbf{M} := (\mathbf{N}\ \ d\mathbf{B}) \tag{3c}$$
$$\mathbf{z}(t) := \begin{pmatrix}\mathbf{v}(\mathbf{c}(t))\\ \mathbf{f}(t)\end{pmatrix} \tag{3d}$$
$$\boldsymbol{\eta}(t) := \begin{pmatrix}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z}(t)\\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{f}(t)\end{pmatrix}. \tag{3e}$$

Please note that we have gathered the unknown signals $\mathbf{v}$ and $\mathbf{f}$ in the vector $\mathbf{z}$. The aim of the following section is to estimate such vector.

3. OBSERVER FOR REACTION RATES AND UNKNOWN INPUTS

Now, in this section we present an observer for $\mathbf{z}(t)$ for systems that comply with the following assumptions.

Assumption 2. Let us consider that

$$n = m + r,$$

which implies that the dimensions of $\mathbf{c}(t)$ and $\mathbf{z}(t)$ are the same.

Assumption 3. In addition, we consider the case in which the time derivative of both $\mathbf{v}(\mathbf{c})$ and $\mathbf{f}(t)$ are element-wise bounded. Thus

$$||\boldsymbol{\eta}(t)||_2 \leq \ell \ \forall t,$$

and we assume ℓ known. In addition, let $\mathbf{M}$ in (3c) be nonsingular.

In the following, the estimated variables are denoted as $\hat{\mathbf{c}}(t)$ and $\hat{\mathbf{z}}(t)$, which are obtained with the following observer.

Proposition 3.1. Consider Assumptions 1, 2, and 3. Then the following dynamical system estimates in finite-time the state $\mathbf{z}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{w}(t) = -k_1\boldsymbol{\phi}_1(\mathbf{e}_c) + k_3\hat{\mathbf{z}}(t) + \left(\mathbf{W} - \mathbf{I_n}\right)\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}\right)\right) \tag{4a}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{z}}(t) = -k_2\boldsymbol{\phi}_2(\mathbf{e}_c), \tag{4b}$$

where

$$\mathbf{e}_c(t) := \hat{\mathbf{c}}(t) - \mathbf{c}(t) \tag{4c}$$
$$\hat{\mathbf{c}}\,(t) = \mathbf{w}(t) + \mathbf{W}\mathbf{c}(t) \tag{4d}$$
$$\mathbf{W} := \mathbf{I_n} - k_3\mathbf{M}^{-1}. \tag{4e}$$

Moreover

$$\boldsymbol{\phi}_1\left(\mathbf{e}_c\right) := \left(\alpha\left|\left|\mathbf{e}_c(t)\right|\right|_2^{-p} + \beta + \gamma\left|\left|\mathbf{e}_c(t)\right|\right|_2^{q}\right)\mathbf{e}_c,\ \ \boldsymbol{\phi}_1\left(\mathbf{0}\right) := \mathbf{0}, \tag{4f}$$

$$\boldsymbol{\phi}_2\left(\mathbf{e}_c\right) := \Big(\alpha(1-p)\left|\left|\mathbf{e}_c(t)\right|\right|_2^{-p} + \beta + \gamma(1+q)\left|\left|\mathbf{e}_c(t)\right|\right|_2^{q}\Big)\boldsymbol{\phi}_1\left(\mathbf{e}_c\right), \tag{4g}$$

where $||\mathbf{e}_c(t)||_2 := \sqrt{\mathbf{e}_c^\top(t)\mathbf{e}_c(t)}$. In addition, $\alpha, \beta, \gamma > 0$, $p = 1/2$, and $q > 0$; furthermore, k_1, k_2, and k_3 are such that the following matrix is Hurwitz

$$\mathbb{A} = \begin{pmatrix}-k_1 & k_3\\ -k_2 & 0\end{pmatrix}. \tag{4h}$$

Additionally

$$\alpha > 2\sqrt{\ell\frac{\overline{\lambda}\left(\mathbb{P}\right)}{\underline{\lambda}\left(\mathbb{Q}\right)}}.$$

□

The proof may be found in Appendix A.

Under the current assumptions, it is remarkable that the observer may recover the reaction rates along with the unknown influx to the system. To attain this, the stoichiometric matrix must be known, which is a reasonable assumption since it can be inferred from the form of the reaction network and the stoichiometric coefficients can be computed by the conversion of species.

The dimension constraint in Assumption 2 is more restrictive since it renders the observer useful for reaction networks whose number of species is equal to the number of reaction rates plus unknown influxes. In the future, we aim to seek to remove such restrictions.

It is also important to note that the matrix $\mathbf{M}$ in (3c) is defined with the dilution rate, which is assumed as positive and constant. In fact, we could allow the dilution rate to be piecewise constant, by computing again the matrix $\mathbf{M}$ whenever the dilution rate is updated and thus updating the observer gain $\mathbf{W}$.

Now, the choice of the particular forms of $\boldsymbol{\phi}_1$ and $\boldsymbol{\phi}_2$ endow the dynamics with a robust, finite-time convergence of the observation error. Moreover, with such a choice both $\hat{\mathbf{c}}(t)$ and $\hat{\mathbf{z}}(t)$ converge to their actual values exactly at the same time; but the presence of noise or an unmodelled perturbation will propagate to all the estimates, despite it being present in only a particular channel, as discussed in (López-Caamal and Moreno, 2015).

4. NUMERICAL SIMULATION

Let us consider the following reaction network

$$S_1 + S_2 \xrightarrow{\nu_1} S_3$$
$$S_1 + S_3 \xrightarrow{\nu_2} S_4$$
$$S_2 \underset{\nu_{3b}}{\overset{\nu_{3f}}{\rightleftharpoons}} 0,$$

along with the reaction rate vector

$$\mathbf{v}(t) = \begin{pmatrix} \nu_1 c_1 c_2 \\ \nu_2 c_1 c_3 \\ \nu_{3f} c_1 - \nu_{3b} \end{pmatrix},$$

with

$$\nu_1 = 0.25$$
$$\nu_2 = 0.75$$
$$\nu_{3f} = 0.1$$
$$\nu_{3b} = 0.2.$$

Here c_i represents the concentration of S_i. Such reaction rates are unknown to the observer. However the stoichiometric matrix is known and has the form

$$\mathbf{N} = \begin{pmatrix} -1 & -1 & 0 \\ -1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

In turn, the input matrix $\mathbf{B}$ is

$$\mathbf{B} = (1\ 0\ 0\ 0)^\top,$$

with the influx

$$f(t) = \max\{0, 2 + 3\tan^{-1}(t/2)\sin(\pi t/2)\exp(-0.3t)\}.$$

Thus, the number of species, n, equals the sum of reaction rates number, m, plus the number of influxes, r.

We also account for a zero gasification vector, i.e., $\mathbf{q}(\mathbf{c}) = \mathbf{0}$, and a dilution rate of $d = 0.1$. With these definitions, one has

$$\mathbf{M} = \begin{pmatrix} -1 & -1 & 0 & 0.1 \\ -1 & 0 & -1 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

which is nonsingular. Thus, by choosing the observer gains

$$\{k_1, k_2, k_3\} = \{3, 2, 1\}$$

one has

$$\mathbf{W} = \begin{pmatrix} 1 & 0 & -1 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 1 & 2 & 1 \\ -10 & 0 & -10 & -19 \end{pmatrix}.$$

By letting $\ell = 100$, one may choose

$$\{\alpha, \beta, \gamma\} = \{18, 2, 5\}\ \{p, q\} = \{0.5, 0.1\}.$$

Figure 1 shows the performance of the estimation of the concentration vector. As one may note, the estimations converge to the actual ones in about 10^{-1} units of time. Although known, by assuming an initial error of the concentration vector, the observer corrects the estimate of both $\mathbf{c}(t)$ and $\mathbf{z}(t)$, which comprise the unknown reaction rates and influx.

In turn, Figure 2 depicts the estimation of the unknown reaction rates, which converge to the actual ones in exactly the same time as the concentration estimates do. This is a trait of the form chosen for the STA.

To finalise, the estimation of the unknown input $f(t)$ is represented in Figure 3.

5. CONCLUDING REMARKS

In this paper, we present an observer for the reaction rate and unknown concentrations in the influx to a CSTR. Such an estimator is capable of providing exact estimates in finite-time for a particular class of reaction networks while requiring the knowledge of the species concentrations, stoichiometric matrix, dilution rate, and gasification vector.

Appendix A. PROOF OF THE OBSERVER IN §3

Proof 1. To estimate the states of System (3), let us consider

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{c}}(t) = -\left(d\mathbf{c}(t) + q\left(\mathbf{c}(t)\right)\right) + \mathbf{M}\mathbf{z}(t) - k_1\boldsymbol{\phi}_1(\hat{\mathbf{c}} - \mathbf{c}) + k_3(\hat{\mathbf{z}} - \mathbf{z}) \tag{A.1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{z}}(t) = -k_2\boldsymbol{\phi}_2(\hat{\mathbf{c}} - \mathbf{c}). \tag{A.1b}$$

The observation error defined as $\mathbf{e}_c(t) := \hat{\mathbf{c}}(t) - \mathbf{c}(t)$ and $\mathbf{e}_z(t) := \hat{\mathbf{z}}(t) - \mathbf{z}(t)$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e}_c(t) = -k_1\boldsymbol{\phi}_1(\mathbf{e}_c) + k_3\mathbf{e}_z(t) \tag{A.2a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e}_z(t) = -k_2\boldsymbol{\phi}_2(\mathbf{e}_c) - \boldsymbol{\eta}(t), \tag{A.2b}$$

which has the form of a generalised multivariable super-twisting algorithm. When appropriately tuned, it exhibits a robust, finite-time stable behaviour (López-Caamal and Moreno, 2019).

The observation error stability may be shown with the Lyapunov function

$$V(t) = \boldsymbol{\zeta}^\top \mathbf{P}\boldsymbol{\zeta}, \tag{A.3}$$

where

$$\boldsymbol{\zeta}(\mathbf{e}_c, \mathbf{e}_z) := \begin{pmatrix} \boldsymbol{\phi}_1(\mathbf{e}_c) \\ \mathbf{e}_z \end{pmatrix}$$

and $\mathbf{P} := \mathbb{P} \otimes \mathbf{I}_n$. In such an expression, the symbol $\otimes$ denotes the Kronecker product and $\mathbb{P} \in \mathbb{R}^{2\times 2}$ satisfies the algebraic Lyapunov Equation

$$\mathbb{P}\mathbb{A} + \mathbb{A}^\top\mathbb{P} = -\mathbb{Q}.$$

The matrices $\mathbb{P}$ and $\mathbb{Q} \in \mathbb{R}^{2\times 2}$ are symmetric and positive-definite; whereas

$$\mathbb{A} := \begin{pmatrix} -k_1 & k_3 \\ -k_2 & 0 \end{pmatrix}$$

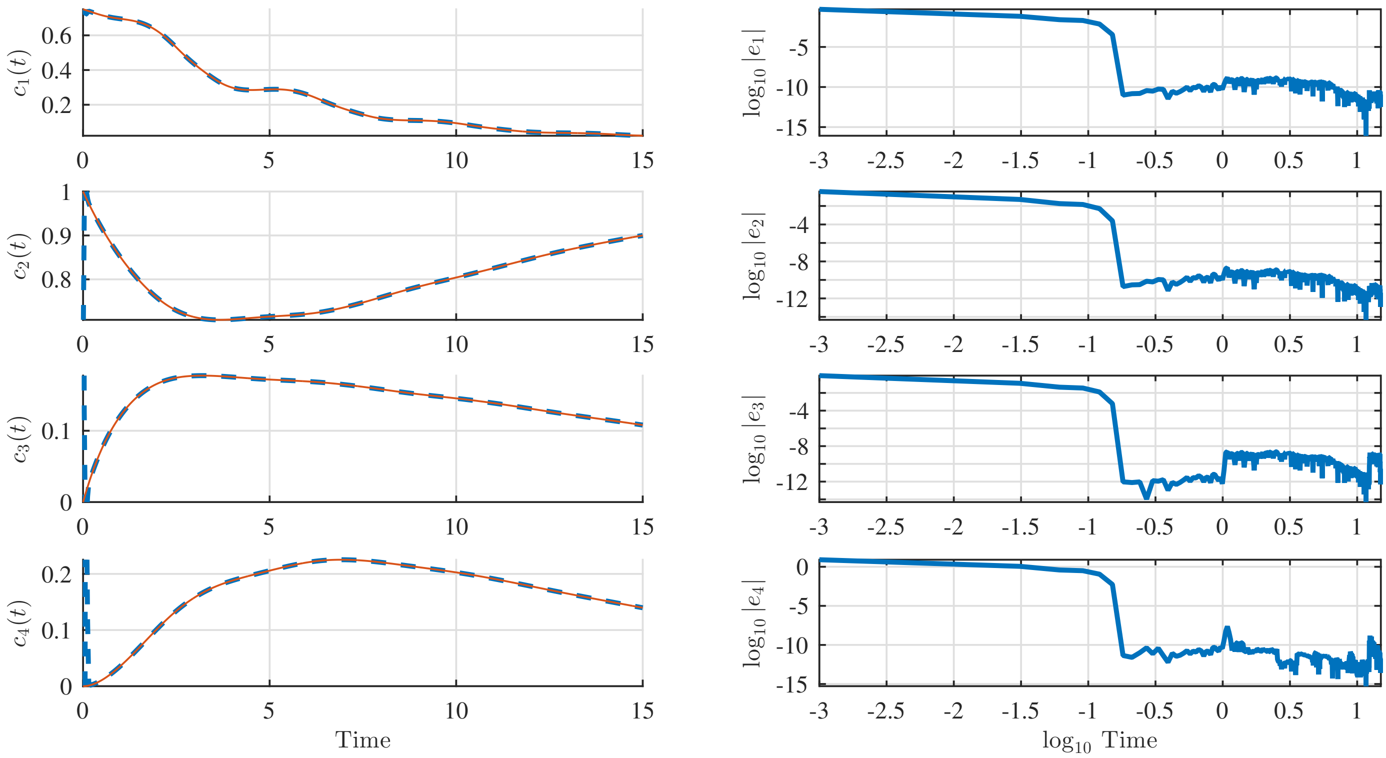

Fig. 1. Actual and estimated states of the reaction network. The red line depicts the actual concentration and the blue line represent the estimate in the left panel and the estimation error in the right one.

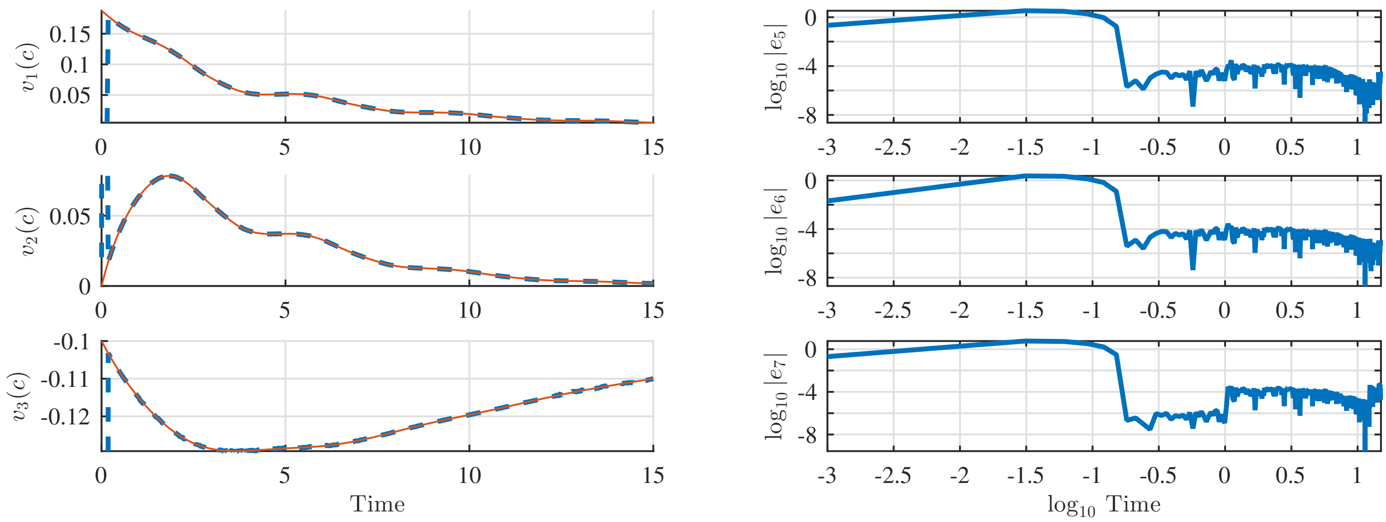

Fig. 2. Estimated reaction rates.

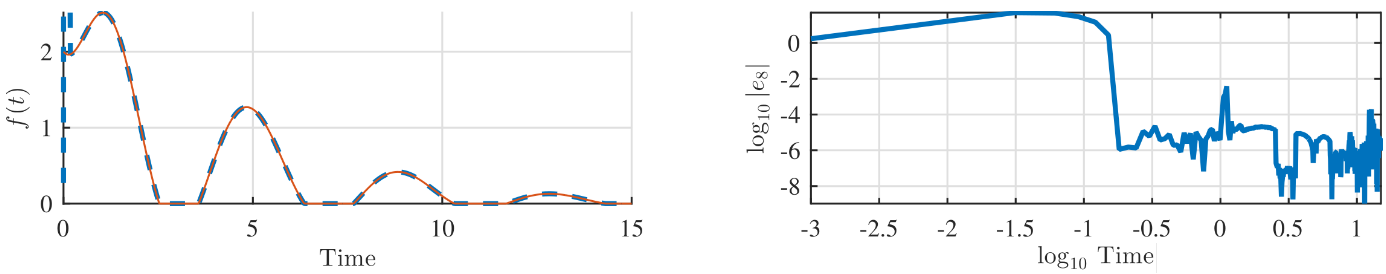

Fig. 3. Estimation of influx concentration $f(t)$.

is Hurwitz. It has been shown that the time derivative of $V(t)$ along (A.2) is given by (López-Caamal and Moreno, 2016, 2019)

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t) = -\boldsymbol{\zeta}^\top\left[\mathbb{Q}\otimes\mathbf{J}(\mathbf{e}_c)\right]\boldsymbol{\zeta} + 2\boldsymbol{\zeta}^\top\mathbf{P}\begin{pmatrix}\mathbf{0}\\ -\boldsymbol{\eta}(t)\end{pmatrix},$$

where

$$\mathbf{J}(\mathbf{e}_c) = \left(\alpha\,||\mathbf{e}_c||_2^{-p} + \beta + \gamma\,||\mathbf{e}_c||_2^{q}\right)\mathbf{I}_n + \left(\gamma q\,||\mathbf{e}_c||_2^{q} - \alpha p\,||\mathbf{e}_c||_2^{-p}\right)\frac{\mathbf{e}_c\mathbf{e}_c^\top}{\mathbf{e}_c^\top\mathbf{e}_c}, \tag{A.4}$$

which is a positive definite, symmetric matrix; whence

$$\underline{\lambda}\left(\mathbf{J}(\mathbf{e}_c)\right) > \frac{\alpha}{2}\,||\mathbf{e}_c||_2^{-1/2}, \tag{A.5}$$

since we have set $p = 1/2$.

Now, in order to ensure the negativity of $\frac{\mathrm{d}}{\mathrm{d}t}V(t)$ one may note that

$$\frac{\mathrm{d}}{\mathrm{d}t}V(t) \le -\underline{\lambda}(\mathbb{Q})\,\underline{\lambda}(\mathbf{J})\,||\boldsymbol{\zeta}||_2^2 + 2\overline{\lambda}(\mathbb{P})\,||\boldsymbol{\zeta}||_2\,||\boldsymbol{\eta}||_2;$$

by using Eq. (A.5) one obtains

$$\begin{aligned}\underline{\lambda}(\mathbf{J})\,||\boldsymbol{\zeta}||_2 \ge& \underline{\lambda}(\mathbf{J})\,\alpha\,||\mathbf{e}_c||_2^{1/2}\\ \ge&\frac{\alpha^2}{2}\,||\mathbf{e}_c||_2^{-1/2}\,||\mathbf{e}_c||_2^{1/2}\\ =&\frac{\alpha^2}{2}.\end{aligned}$$

Thus,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}V(t) \le& -\left(\frac{\alpha^2}{2}\underline{\lambda}(\mathbb{Q}) - 2\overline{\lambda}(\mathbb{P})\,||\boldsymbol{\eta}||_2\right)||\boldsymbol{\zeta}||_2\\ \le& -\left(\frac{\alpha^2}{2}\underline{\lambda}(\mathbb{Q}) - 2\overline{\lambda}(\mathbb{P})\,\ell\right)||\boldsymbol{\zeta}||_2.\end{aligned}$$

Hence to ensure negativity one must choose

$$\alpha > 2\sqrt{\ell\frac{\overline{\lambda}(\mathbb{P})}{\underline{\lambda}(\mathbb{Q})}}.$$

So far, the stability of the observation error has been established. However, the observer (A.1) requires the use of $\mathbf{z}(t)$, which is unknown. It can, nevertheless, be written in terms of the known vector $\mathbf{c}(t)$ from (3a) as

$$\mathbf{z}(t) = \mathbf{M}^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}(t) + d\mathbf{c}(t) + \mathbf{q}(\mathbf{c}(t))\right).$$

By using this last Equation in (A.1a) one obtains

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{c}}(t) =& -\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}(t)\right)\right) - k_1\boldsymbol{\phi}_1(\mathbf{e}_c)\\ &+ k_3\hat{\mathbf{z}}(t) + (\mathbf{M} - k_3\mathbf{I_n})\mathbf{z}(t)\\ =& -\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}(t)\right)\right) - k_1\boldsymbol{\phi}_1(\mathbf{e}_c) + k_3\hat{\mathbf{z}}\\ &+ \mathbf{W}\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}(t) + d\mathbf{c}(t) + \mathbf{q}(\mathbf{c}(t))\right)\\ \frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{\mathbf{c}}(t) - \mathbf{W}\mathbf{c}(t)\right) =& -\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}(t)\right)\right) - k_1\boldsymbol{\phi}_1(\mathbf{e}_c)\\ &+ k_3\hat{\mathbf{z}}(t) + \mathbf{W}\left(d\mathbf{c}(t) + \mathbf{q}(\mathbf{c}(t))\right)\\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{w}(t) =& -k_1\boldsymbol{\phi}_1(\mathbf{e}_c) + k_3\hat{\mathbf{z}}(t)\\ &+ \left(\mathbf{W} - \mathbf{I_n}\right)\left(d\mathbf{c}(t) + \mathbf{q}\left(\mathbf{c}(t)\right)\right),\end{aligned}$$

which completes the proof.

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