DESIGN AND PRACTICAL USE OF PROBABILISTIC OBSERVERS FOR MASS-BALANCE BASED BIOPROCESS MODELS

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Abstract: In this paper, the design of probabilistic observers for mass-balance based bioprocess models is investigated. It is assumed that the probability density function of every uncertain parameter, input and/or initial state is known *a priori*. Then, the probability density functions of the state variables are obtained, at any time, by considering the image of this initial probability density function by the flow of the dynamical system. In comparison to classical open-loop interval observers, the method provides information on the confidence level of the estimates rather than simple upper and lower bounds. The numerical implementation of the method is closely considered and an application to an industrial anaerobic digester is detailed.

Keywords: non-linear estimation, unknown inputs, uncertain parameters, mass-balance models, bioprocesses, anaerobic digestion.

1. INTRODUCTION

One of the main difficulties in the monitoring and control of biological reactors lies in the absence, in most applications, of cheap and reliable sensors capable of providing direct, on-line measurements of the biological state variables. The design of *observers* for online monitoring of the state variables which are not measurable in real time has thus received much attention in the literature, and has given rise to numerous practical applications [Bastin and van Impe, 1995].

Bioprocess models generally consist of two parts: (*i*) a part based on mass-balance considerations which requires few phenomenological knowledge; (*ii*) another part that describes the biological reactions (kinetics) and therefore includes a large part of phenomenological knowledge. This later part introduces large uncertainties in the models, and it is well-known that

the classical observers such as the extended Kalmann filter and the high gain observer [Gauthier et al., 1992, Bernard et al., 1998] may exhibit a poor convergence rate or even fail to converge. Taking advantage of the special model structure, *asymptotic observers* have been proposed which do not require the knowledge of the kinetics [Bastin and Dochain, 1990]. More recently, *interval observers* have been designed in order to deal with these uncertainties [Rapaport and Gouzé, 2003]. The idea is to estimate rigorous intervals for the state variables by considering conservative bounds on the uncertainties (such as imprecisions in the influent measurements or model parameters). This requires to weaken the observation principle in the sense that the observation error is no longer expected to asymptotically converge to zero. Several applications have been successfully considered for biological systems [*e.g.* Gouzé et al., 2000]. But even if interval observers are more robust than the aforementioned asymptotic ob-

servers, poor information is obtained on the estimates since "only" guaranteed upper and lower bounds are derived.

In many situations however, more information than simple upper and lower bounds is available on the uncertainties, *e.g.*, their probability density functions (p.d.f.). For the uncertain parameters in particular, confidence intervals can be easily obtained from the application of a parameter identification procedure. In this work, we extend the concept of interval observers by developing *probabilistic observers* which estimate the probability density functions of the unmeasured states. Major differences between the proposed observers and the extended Kalman filter are that no assumption is stated here for the kinetic expressions and that aribitrary p.d.f.s can be selected for the uncertain parameters.

The paper is organised as follow: some results on both asymptotic and interval observers are first recalled in section 2; probabilistic observers are considered in section 3 for general mass-balance bioprocess models, and their numerical implementation is closely considered; the method is illustrated in section 4 by a practical application of a probabilistic observer to estimate the COD concentration in an industrial anaerobic digester.

2. ASYMPTOTIC AND INTERVAL OBSERVERS FOR BIOPROCESSES

A bioprocess operated in a stirred tank bioreactor is often described by means of general mass-balance based models of the following form [Bastin and Dochain, 1990]:

$$\dot{\boldsymbol{\xi}} = \mathcal{K}\boldsymbol{r}\left(\boldsymbol{\xi}\right) + D\left(\boldsymbol{\xi}^{in} - \boldsymbol{\xi}\right) - \boldsymbol{q}\left(\boldsymbol{\xi}\right) \qquad (1)$$

where $\boldsymbol{\xi} \in \mathbb{R}^{n_\xi}$ (resp. $\boldsymbol{\xi}^{in}$) denotes the concentration vector in the liquid phase (resp. in the influent), $\mathcal{K} \in \mathbb{R}^{n_\xi \times n_r}$ the yield coefficient matrix, $\boldsymbol{r} \in \mathbb{R}^{n_r}$ the reaction rate vector, $\boldsymbol{q} \in \mathbb{R}^{n_\xi}$ the gaseous exchange vector, and $D \in \mathbb{R}$ the dilution rate.

Throughout the paper, it is assumed that $(n_\xi - n_b)$ components of the state variables are measured on-line with $n_\xi - n_b \geq n_r$, and we denote $\boldsymbol{\xi_a} \in \mathbb{R}^{n_\xi - n_b}$, $\boldsymbol{\xi_b} \in \mathbb{R}^{n_b}$ the measured and unmeasured state variables respectively. It is also assumed that the gaseous flow rates $\boldsymbol{q}$ are measured on-line. It follows that Eq. (1) can be rephrased as:

$$\dot{\boldsymbol{\xi}}_a = \mathcal{K}_a \boldsymbol{r}\left(\boldsymbol{\xi}\right) + D\left(\boldsymbol{\xi}_a^{in} - \boldsymbol{\xi}_a\right) - \boldsymbol{q}_a\left(\boldsymbol{\xi}\right) \qquad (2)$$

$$\dot{\boldsymbol{\xi}}_b = \mathcal{K}_b \boldsymbol{r}\left(\boldsymbol{\xi}\right) + D\left(\boldsymbol{\xi}_b^{in} - \boldsymbol{\xi}_b\right) - \boldsymbol{q}_b\left(\boldsymbol{\xi}\right) \qquad (3)$$

with $(\mathcal{K}_a, \mathcal{K}_b)$, $\left(\boldsymbol{\xi}_a^{in}, \boldsymbol{\xi}_b^{in}\right)$ and $(\boldsymbol{q}_a, \boldsymbol{q}_b)$ being the induced partition of $\mathcal{K}$, $\boldsymbol{\xi}^{in}$ and $\boldsymbol{q}$ respectively.

We state the following hypothesis:

Hypothesis 1. Matrix $\mathcal{K}_a \in \mathbb{R}^{(n_\xi - n_b) \times n_r}$ has full rank.

From hypothesis 1 and a linear change of variables, the following n_b-dimensional auxiliary system can be derived:

$$\dot{\boldsymbol{z}} = -D\left(\boldsymbol{z} - \boldsymbol{z}^{in}\right) - \mathcal{P}\boldsymbol{q}_a - \boldsymbol{q}_b \qquad (4)$$

$$\boldsymbol{\xi}_b = \boldsymbol{z} - \mathcal{P}\boldsymbol{\xi}_a \qquad (5)$$

where: $\mathcal{P} \triangleq -\mathcal{K}_b \mathcal{K}_a^\dagger$

and $\mathcal{K}_a^\dagger$ is a left inverse of $\mathcal{K}_a$. Note in particular that, in the auxiliary system (4,5), the measured variable $\boldsymbol{\xi_a}$ is used as an input.

The following result holds.

Lemma 1. Under Hypothesis 1 (and provided D is persistently exiting), the solution $\hat{\boldsymbol{\xi}}_b$ of the following open-loop observer converges asymptotically towards the solution $\boldsymbol{\xi}_b$ of the reduced system (3):

$$\dot{\hat{\boldsymbol{z}}} = -D\left(\hat{\boldsymbol{z}} - \boldsymbol{z}^{in}\right) - \mathcal{P}\boldsymbol{q}_a - \boldsymbol{q}_b \qquad (6)$$

$$\hat{\boldsymbol{\xi}}_b = \hat{\boldsymbol{z}} - \mathcal{P}\boldsymbol{\xi}_a \qquad (7)$$

Proof. see, *e.g.*, Bastin and Dochain [1990]. □

Such observers have however several defects due to their open-loop nature. In particular, it is implicitly assumed that the mass-balance part of the model is perfectly known and that neither the measurements, nor the values of the feeding inputs, nor the estimates of the yield coefficients (matrix $\mathcal{K}$) are biased. Otherwise, the predictions of the mass-balance based observer (6,7) will be corrupted and might provide poor estimates of the unmeasured concentrations $\boldsymbol{\xi}_b$.

In the case of large uncertainties, it is no longer possible to build exact observers guarantying that the observation errors converges to zero. Therefore, the observation principle must be revisited and the results must be weakened. A complementary approach, called interval observers, provides guaranteed enclosures on the estimated states, whenever upper and lower bounds are known on the uncertain inputs and parameters. Such observers consist in coupling two estimators providing each an over-estimate $\boldsymbol{x}^+\left(t\right)$ and an under-estimate $\boldsymbol{x}^-\left(t\right)$ of the unknown state variables $\boldsymbol{x}\left(t\right)$ at any time. Details on interval observers can be found, *e.g.*, in Gouzé et al. [2000], Rapaport and Gouzé [2003].

The following proposition applies the concept of interval observers to the auxiliary system (4) derived from the general mass-balance based model (1).

Proposition 1. The following pair of systems is an interval observer for the variables $z\left(t\right)$ solution of (4):

$$\dot{\boldsymbol{z}}^+ = -D\boldsymbol{z}^+(t) + D\boldsymbol{z}^{in^+}(t)$$
$$-\mathcal{P}^-\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right)\boldsymbol{q}_a(t) + \boldsymbol{q}_b(t)$$
$$\dot{\boldsymbol{z}}^- = -D\boldsymbol{z}^-(t) + D\boldsymbol{z}^{in^-}(t)$$
$$-\mathcal{P}^+\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right)\boldsymbol{q}_a(t) + \boldsymbol{q}_b(t)$$
$$\text{with: } \boldsymbol{z}^+(0) = \boldsymbol{\xi}_b^+(0) + \mathcal{P}^+\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right)\boldsymbol{\xi}_a(t)$$
$$\boldsymbol{z}^-(0) = \boldsymbol{\xi}_b^-(0) + \mathcal{P}^-\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right)\boldsymbol{\xi}_a(t)$$

where the unknown parameters $\boldsymbol{p} \in \mathbb{R}^{n_p}$ and inputs $\boldsymbol{z}^{in} \in \mathbb{R}^{n_b}$ are characterised by their upper and lower bounds:

$$p_j^- \le p_j \le p_j^+ \ , \ \forall j = 1 \dots n_p$$
$$z_i^{in^-}(t) \le z_i^{in}(t) \le z_i^{in^+}(t) \ , \ \forall t, \ \forall i = 1 \dots n_b$$

and the upper and lower bound matrices $\mathcal{P}^+, \mathcal{P}^-$ are defined componentwise:

$$\mathcal{P}_{i,j}^-\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right) \le \mathcal{P}_{i,j}(\boldsymbol{p}) \le \mathcal{P}_{i,j}^+\left(\boldsymbol{p}^+, \boldsymbol{p}^-\right) \ ,$$
$$\forall \boldsymbol{p} \in \left[\boldsymbol{p}^-, \boldsymbol{p}^+\right] \ , \ \forall i = 1 \dots n_b \ , \ j = 1 \dots n_\xi - n_b$$

Proof. See, *e.g.*, Rapaport and Gouzé [2003]. □

Interval observers provide guaranteed bounds on the estimation of the unmeasured variables, given rigorous bounds on the parameters and the inputs. However, the resulting intervals might be large if the uncertainty is high. In this case, it could be interesting to build subintervals on the estimates corresponding to different confidence levels on the uncertainty. Tools to derive such observers are discussed in the next section.

3. PROBABILISTIC OBSERVERS

As mentioned before, it is not rare that the influent concentrations and/or model parameters are not known precisely for biological processes. For parameters in particular, estimates as well as confidence intervals can be obtained under the application of a parameter identification procedure. More knowledge than simple upper and lower bounds can obviously be obtained on the unmeasured state variables, *e.g.* the probability distribution of the estimates.

3.1 Mathematical background

In mass-balance based bioprocess models of the form (1), the uncertainties may correspond to the yield coefficients in matrix $\mathcal{K}$, to the influent concentrations $\boldsymbol{\xi}^{in}$, and/or to the unmeasured state variables at initial time $\boldsymbol{\xi}_{b0}$. In addition, the measurements of the state variables $\boldsymbol{\xi}_a$ and the gaseous flow rates $\boldsymbol{q}_a$, $\boldsymbol{q}_b$ might be noisy. In order to derive the p.d.f.s of the unmeasured state variables $\boldsymbol{\xi}_b$, we consider the auxiliary dynamical system (4,5) defined in section 2.

Hypothesis 2. The auxiliary dynamical system (4,5) falls into the following class of dynamical systems:

$$(\mathcal{S}) \quad \begin{cases} \dot{\boldsymbol{z}}(t) = \mathcal{A}(\boldsymbol{p}, t)\,\boldsymbol{z}(t) + \boldsymbol{b}(\boldsymbol{p}, t) \\ \boldsymbol{\xi}_b(t) = \boldsymbol{z}(t) + \boldsymbol{c}(\boldsymbol{p}, t) \\ \boldsymbol{z}(0) = \boldsymbol{\xi}_b(0) - \boldsymbol{c}(\boldsymbol{p}, 0) \end{cases}$$

where $\boldsymbol{p} = \left(p_1, \dots, p_{n_p}\right)^t \in \mathbb{R}^{n_p}$ denotes the vector of the uncertain parameters, and the components of $\mathcal{A} \in \mathbb{R}^{n_b \times n_b}$, $\boldsymbol{b} \in \mathbb{R}^{n_b}$ and $\boldsymbol{c} \in \mathbb{R}^{n_b}$ are $\mathcal{C}^1$ with respect to $p_1, \dots, p_{n_p}$. In addition, the uncertain parameters $\boldsymbol{p}$ and initial conditions $\boldsymbol{z}_0$ have *independent* p.d.f.s.

Remark 1. For sake of simplicity, we consider that parameters $p_1, \dots, p_{n_p}$ are constants with known p.d.f..

Notations 1. In the sequel, the following notations are used: $\chi_0 = \left(\boldsymbol{\xi}_{b0}^t, \boldsymbol{p}^t\right)$, $\mathcal{Z}_0 = (\boldsymbol{z}_0^t, \boldsymbol{p}^t)$, $\chi_t = \left(\boldsymbol{\xi}_{bt}^t, \boldsymbol{p}^t\right)$ and $\mathcal{Z}_t = (\boldsymbol{z}_t^t, \boldsymbol{p}^t)$. In addition, we denote f_{χ_0}, $f_{\mathcal{Z}_0}$, f_{χ_t} and $f_{\mathcal{Z}_t}$ their respective p.d.f..

The estimation of the p.d.f. of the unmeasured state variables $\boldsymbol{\xi}_b$ at a given time t can be decomposed into three successive steps:

1) estimate the p.d.f. of the random variable $\mathcal{Z}_0$ at initial time, from the individual p.d.f. of the unmeasured state variables $\boldsymbol{\xi}_{b0}$ and the uncertain parameters $\boldsymbol{p}$;
2) compute the image $f_{\mathcal{Z}_t}$ at time t of the p.d.f. of $f_{\mathcal{Z}_0}$, by the flow of the auxiliary dynamical system (4);
3) estimate the p.d.f. of the unmeasured state variables $\boldsymbol{\xi}_{bt}$ at time t, from the p.d.f. of $\mathcal{Z}_t$.

The following Theorem [see, *e.g.*, Grimmett and Stirzaker, 2001] provides a general framework to calculate the image of a given p.d.f. by a $\mathcal{C}^1$-diffeomorphism for each aforementioned step.

Theorem 1. Let $\mathcal{U}$, $\mathcal{V}$ be open subsets of $\mathbb{R}^n$, K be a compact subset of U, and $\phi : \mathcal{U} \longmapsto \mathcal{V}$ be a $\mathcal{C}^1$ diffeomorphism. If z is a random variable with a p.d.f. f_z, then the random variable $\omega = \phi(z)$ has a p.d.f. f_ω given by:

$$f_\omega(\omega) = \begin{cases} f_z\left(\phi^{-1}(\omega)\right)\det\left(J_{\phi^{-1}}(\omega)\right) & \text{if } \omega \in \phi(K) \\ 0 & \text{otherwise} \end{cases}$$

where J_ϕ denotes the Jacobian matrix of ϕ.

For steps 1) and 3), let the mapping ψ_t be defined as:

$$\psi_t : \mathcal{U}_t' \longrightarrow \mathcal{U}_t = \psi_t(\mathcal{U}_t')$$
$$\mathcal{Z}_t \longmapsto \chi_t = \left(\boldsymbol{\xi}_{bt}^t, \boldsymbol{p}^t\right)^t$$

where $\mathcal{U}_t'$ is an open subset of $\mathbb{R}^{n_b + n_p}$. From Hypothesis 2, the following property is immediate.

Property 1. ψ_t is a $\mathcal{C}^1$-diffeomorphism.

For step 2), consider the mapping φ_0^t defined as:

$$\varphi_0^t \; : \; \mathcal{U}_0' \longrightarrow \mathcal{U}_t' = \varphi_0^t \left(\mathcal{U}_0\right)$$
$$\mathcal{Z}_0 \longmapsto \mathcal{Z}_t = \left(\boldsymbol{z}_t^t, \boldsymbol{p}^t\right)^t$$

with $\mathcal{U}_0'$ being an open subset of $\mathbb{R}^{n_b+n_p}$. The mapping φ_0^t can be explicitly defined. Indeed, from linear systems theory, a general solution of system $(\mathcal{S})$ can be obtained from:

$$\boldsymbol{z}_t = \Phi\left(0,t,\boldsymbol{p}\right)\boldsymbol{z}_0 + \int_0^t \Phi\left(\tau,t,\boldsymbol{p}\right)\boldsymbol{b}\left(\tau,\boldsymbol{p}\right)\,d\tau \; (8)$$

where $\Phi\left(\cdot,\cdot,\boldsymbol{p}\right) \in \mathbb{R}^{n_b \times n_b}$ is the transition matrix, *i.e.* the solution of the matrix differential equation:

$$\frac{d}{dt}\Phi\left(\tau,t,\boldsymbol{p}\right) = \mathcal{A}\left(t,\boldsymbol{p}\right)\Phi\left(\tau,t,\boldsymbol{p}\right) \; , \; \forall t$$
$$\Phi\left(\tau,\tau,\boldsymbol{p}\right) = I_{n_b \times n_b}$$

Based on the analytical solution of system $(\mathcal{S})$ and Hypothesis 2, it can be shown that the following property holds:

Property 2. φ_0^t is a $\mathcal{C}^1$-diffeomorphism.

Proposition 2. The p.d.f. f_{χ_t} corresponding to the image $\chi_t = \left(\boldsymbol{\xi}_{\boldsymbol{b}_t}^t, p^t\right)^t$ of the random variable $\chi_0 \in K_0 \subset \mathcal{U}_0$ is given by:

$$f_{\chi_t}\left(\chi_t\right) = \begin{cases} \dfrac{f_{\chi_0}\left(\psi_0 \circ \varphi_0^{t\,-1} \circ \psi_t^{-1}\left(\chi_t\right)\right)}{\det\,\Phi\left(0,t,\boldsymbol{p}\right)} \\ \qquad \text{if} \quad \chi_t \in K_t = \varphi_0^t\left(K_0\right) \\ \\ 0 \quad \text{otherwise} \end{cases}$$

Proof. From Properties 1 and 2, the transformations in steps 1), 2) and 3) are $\mathcal{C}^1$-diffeomorphisms. The overall transformation $\psi_0 \circ \varphi_0^{t\,-1} \circ \psi_t^{-1}$ is therefore a $\mathcal{C}^1$-diffeomorphism (chain rule of differentiation), and Theorem 1 applies. Since,

$$\det\,J_{\psi_0} = \det\,J_{\psi_t} = I_{n_b+n_p}$$

then,

$$\det\,J_{\left(\psi_0 \circ \varphi_0^{t\,-1} \circ \psi_t^{-1}\right)} = \det\,J_{\varphi_0^{t\,-1}}$$

In addition,

$$\det\,J_{\varphi_0^t} = \det\begin{pmatrix} \Phi\left(0,t,\boldsymbol{p}\right) & \star \\ 0_{n_p \times n_b} & I_{n_p \times n_p} \end{pmatrix} = \det\,\Phi\left(0,t,\boldsymbol{p}\right)$$

which completes the proof. $\qquad\square$

Finally, individual p.d.f.s for the unmeasured state variables $\boldsymbol{\xi}_b$ can be obtained, at any time t, by integrating the joint state/parameter p.d.f. with respect to the uncertain parameters $\boldsymbol{p}$. Also note that the aforementionned procedure does not require any particular assumption for the initial state/parameter p.d.f.s, and is therefore not restricted to unimodal p.d.f.s.

3.2 Numerical implementation and practical application

In the sequel, we restrict ourselves to the subclass of dynamical systems $(\mathcal{S})$ for which the matrix $\mathcal{A}$ is Hurwitz. Otherwise the dynamical system would be unstable, which is unrealistic here since $(\mathcal{S})$ is intended to be used as an auxiliary system/observer of the stable BIBO class of models (1).

The numerical implementation of the previous framework can be decomposed into two successive steps:

1) Compute the image of the joint p.d.f. by the diffeomorphism $\psi_0 \circ \varphi_0^{t\,-1} \circ \psi_t^{-1}$. This can be done, *e.g.*, by defining a grid in the joint state/parameter space. Note that due to the linearity of the dynamical system in the state variables, it is only necessary to integrate the trajectories of the dynamical system $(\mathcal{S})$ at the edges of the state variation range; for fixed values of the parameters, evenly spaced points in the initial grid indeed remain evenly spaced at any time (see Eq. (8)).
2) Integrate the joint state/parameter p.d.f. at a given time t, with respect to the parameters, in order to obtain individual p.d.f.s for the state variables.

It should be stressed that step 2) is by far the most complex and time consuming step in the procedure. As the influence of the initial conditions $\boldsymbol{z}_0$ vanish with increasing time, the joint p.d.f. tends to degeneracy (it becomes infinitely thin), and eventually results in inaccurate p.d.f.s. This can however be easily detected in pratice, *e.g.*, by monitoring the error $\varepsilon = \left|1 - \int_{K_t} f_{\chi_t} d\chi_t\right|$. The degeneracy of the joint p.d.f. is illustrated in the example below.

ILLUSTRATIVE EXAMPLE – To illustrate the practical difficulties encountered when attempting to implement the probabilistic observer numerically, we consider the following simple dynamic system

$$\begin{cases} \dot{z}\left(t\right) = -z\left(t\right) + p \; , \; \forall t > 0 \\ z\left(0\right) = z_0 \end{cases} \qquad (\mathcal{T})$$

and assume that either p.d.f. of z_0 and p are normal distributions, denoted $\mathcal{N}\left(\overline{z_0}, \sigma_{z_0}\right)$ and $\mathcal{N}\left(\overline{p}, \sigma_p\right)$ respectively. Then applying Proposition 2 allows us to compute the joint p.d.f. of $\mathcal{Z}_t = \left(z_t, p\right)^t$ at a given time $t > 0$ as

$$f_{\mathcal{Z}_t}\left(\mathcal{Z}\right) = \frac{f_{\mathcal{Z}_0}\left(\varphi_0^{t\,-1}\left(\mathcal{Z}\right)\right)}{\det\,\Phi\left(0,t\right)}$$

where

$$\Phi\left(0,t\right) = \mathrm{e}^{t-t_0}$$

$$f_{\mathcal{Z}_0}\left(\mathcal{Z}\right) = \frac{1}{2\pi\sigma_{z_0}\sigma_p}\mathrm{e}^{-\frac{1}{2}\left[\left(\frac{z-\overline{z_0}}{\sigma_{z_0}}\right)^2+\left(\frac{p-\overline{p}}{\sigma_p}\right)^2\right]}$$

$$\varphi_0^{t\,-1}\left(\mathcal{Z}\right) = \begin{pmatrix} \mathrm{e}^{t-t_0}z + \left[1 - \mathrm{e}^{t-t_0}\right]p \\ p \end{pmatrix}$$
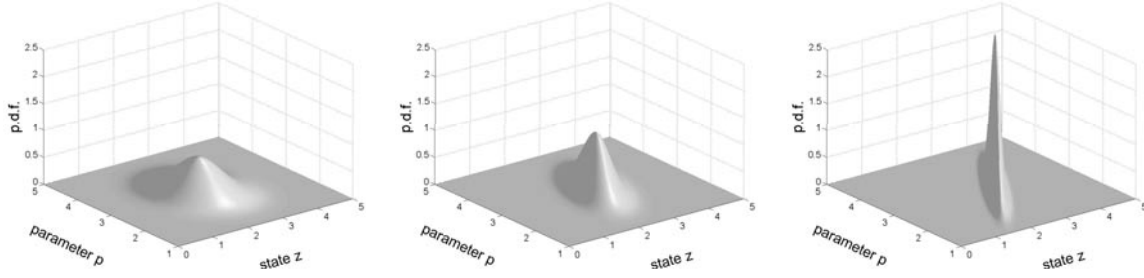
Figure 1. Evolution of the joint state/parameter p.d.f. *Left plot*: $t = 0$; *Middle plot*: $t = 0.5$; *Right plot*: $t = 1.5$.

for any $\mathcal{Z} = (z, p)^t$. By combining these expressions and letting t tend to infinity, it can be proved that

$$f_{\mathcal{Z}_t}(\mathcal{Z}) \xrightarrow{t \longrightarrow +\infty} +\infty \ , \ \text{if } z = p$$
$$f_{\mathcal{Z}_t}(\mathcal{Z}) \xrightarrow{t \longrightarrow +\infty} 0 \qquad , \ \text{otherwise}$$

This is illustrated in Fig. 1. $\qquad\qquad\square$

It is frequent, from a monitoring point of view, that the key state variables are measured at a low frequency from off-line analysis in order to check for proper process operation (*e.g.*, once a week in anaerobic digesters for COD and VSS). Accordingly, the approach used in this work to avoid the aforementionned numerical problems consists in repeatedly reseting the observer from a periodic process sampling. For practical applications where the observer cannot be reseted, it is beleived that the numerical difficulties could be circumvented by adding an artificial term acting as a *diffusion* term [see, *e.g.*, Zeeman, 1988]; this will be the topic of future research.

4. CASE STUDY

A simple model of the anaerobic digestion process is considered by accounting for a single substrate (COD) and a single bacterial population, denoted s and x respectively. The biological reaction is represented as

$$k \, s \xrightarrow{r(\boldsymbol{\xi}) = \mu(\cdot) \, x} x$$

where k is a yield coefficient, and $\mu(\cdot)$ represents the bacterial growth rate. By assuming perfect mixing in the digester, the following 2-dimensional dynamical model is obtained

$$\dot{x}(t) = -D(t)\, x(t) + \mu(\cdot)\, x(t) \qquad (9)$$
$$\dot{s}(t) = -D(t)\, \big(s(t) - s^{in}(t)\big) - k\,\mu(\cdot)\, x(t)$$

where $s^{in}(t)$ stands for the concentration of substrate in the feeding stream. In addition, the methane flow rate is defined as $q_{CH_4}(t) = k'\,\mu(\cdot)\, x(t)$ with k' being the yield coefficient associated to methane production.

Based on model (9), the following auxiliary system can be derived for the biomass concentration provided that the methane gaseous flow rate as well as the influent COD are measured on-line

$$\dot{\hat{s}}(t) = -D(t)\,\hat{s}(t) + \left[D(t)\, s^{in} - \frac{k}{k'}\, q_{CH_4}(t) \right] \quad (10)$$

Experimental data from a $2{,}000\ \mathrm{m}^3$ industrial digester located at Agralco Ltd. in Estella, Spain, are considered. The digester is fed with wine distillery vinasses, and the measurements consist of the dilution rate D and the methane outflow rate q_{CH_4} at a high sampling frequency over more than $140\ \mathrm{days}$. In our objective to design a probabilistic observer for estimating the COD concentration based on Eq. (10), we consider the uncertainties on (i) the parameter $\gamma = \frac{k}{k'}$, (ii) the influent concentration s^{in} and, (iii) the COD concentration s_0 at initial time.

- The value of γ was estimated off-line based on mass-balance considerations along with its standard deviation: $\gamma = 5.30\ 10^{-2} \pm 0.98\%$. It is assumed that the p.d.f. for this parameter is Gaussian.
- The uncertainty on s^{in} is handled by considering a multiplicative noise ε defined as $s^{in}(t) = \overline{s^{in}}\,(1 + \varepsilon(t))\,, \forall t$. It was found from experimental data that $\overline{s^{in}} = 35.9\,\mathrm{g.L}^{-1}$ and that the p.d.f. of ε can be assimilated to a normal distribution $\mathcal{N}(0, \sigma_\varepsilon)$ with $\sigma_\varepsilon = 0.124$.
- In accordance to the discussion in subsection 3.2, the observer is reinitialised every one week by considering off-line COD measurements; the p.d.f. of these initial concentrations $z_k = z^{\exp}(t_k)$ are assumed to be uniform in the range $z_k \pm 20\%$.

Also note that the experimental data have been filtered and, for the sake of simplicity, no measurement error is taken into account here for D and q_{CH_4}.

A probabilistic observer can be derived for the COD concentration from Eq. (10) by applying Proposition 2. In this case, note that $\psi_t = \psi_0^{-1} = I$ and $\Phi(\tau, t) = \exp\left[-\int_\tau^t D(s)\,ds \right]$. The resulting p.d.f. of the estimate $\hat{s}$ are plotted in Fig. 2 (upper plot) at different time instants. Experimental points are also displayed for the sake of comparison. Note that the variation range of $\hat{s}$ (corresponding to the vertical segments) is rather conservative, but a significant part of the range has a null probability. Also note that the experimental points are correctly enclosed within
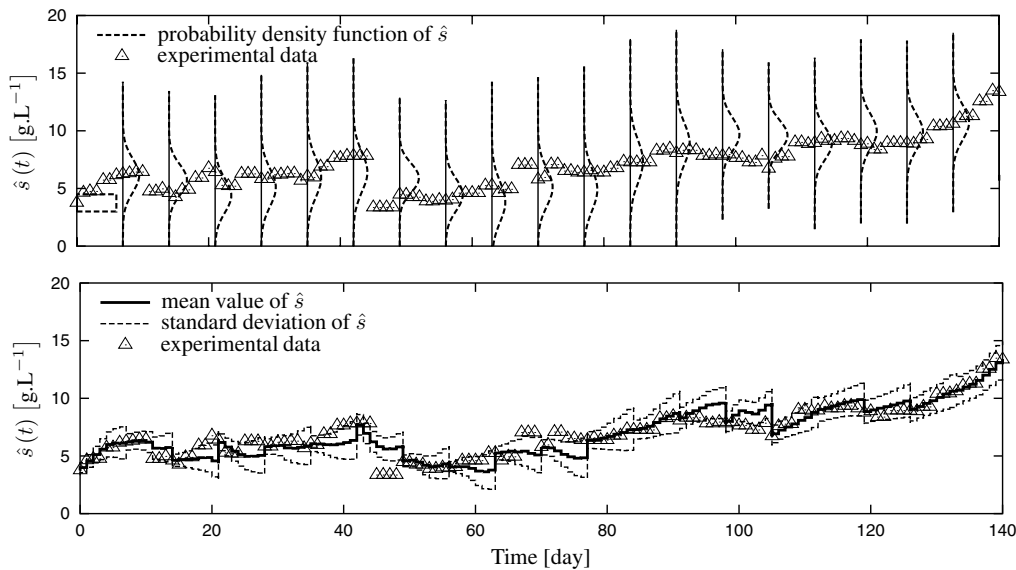
Figure 2. Estimated COD concentration in the digester. *Upper plot*: Probability density function. *Lower plot*: Mean value and standard deviation.

the non-null probability part, and that the maximum likelihood estimate is close to the experimental points.

A straightforward interpretation for the p.d.f. can be obtained by extracting the mean and standard deviation values of $\hat{s}$. These values are pictured in Fig. 2 (lower plot). It can be seen in particular that the estimates are close to the experimental measurements, and the interval corresponding to the standard deviation of $\hat{s}$ mainly encloses these measurements. From a sensitivity point of view, the quality of the standard-deviation based bounds is strongly affected by the p.d.f. of parameter γ, while the influence of the initial p.d.f. after the observer is reseted rapidly vanishes and therefore remains limited.

5. CONCLUSIONS

In this paper, the design of probabilistic observers was investigated for general mass-balance based bioprocess models. It was shown how the probability density functions of the unmeasured state variables can be derived from the knowledge of the probability density functions of the uncertain parameters and the measurement noises. An application of the method to the estimation of the COD concentration in an industrial anaerobic digester was then presented, which demonstrate the tractability and good performances of the approach.

Although only an asymptotic rate of convergence is guaranteed in this paper, it is worth pointing out that this rate can be chosen in some cases [Rapaport and Gouzé, 2003]. Such probabilistic observers can therefore be used as tools to improve bioprocess monitoring. In addition, they could also be applied in the scope of bioprocess supervision and fault detection,

e.g., by defining a given tolerance expressed in term of a threshold confidence level.

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