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# Dynamic estimation of specific growth rates and concentrations of bacteria for the anaerobic digestion

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**Abstract:** The paper proposes an observability analysis and estimation schemes for specific growth rates and biomass concentrations of the anaerobic digestion process. A 3-stage model of 5 dynamic states is assumed, describing the hydrolysis, acidogenesis and methanogenesis of two different populations of microorganisms (acidogenic and methanogenic). The main result is that the specific growth rates of the two populations of bacteria can be stability estimated only from easily measured quantities – the dilution rate and the flow rates of methane and carbon dioxide in the biogas. The estimation schemes thus obtained have quite interesting features one of which is their freeness of most yield coefficients often hard to identify. The analysis rests on the differential algebraic approach of observation problems. The results are being verified currently with experimental data from a 100 m<sup>3</sup> pilot bioreactor fed with cattle dung. Realistic simulations are presented in this paper as illustrations of the estimator performance.

Keywords: Waste treatment, Biotechnology, Observer, Estimation theory, Algebraic systems theory

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## 1. INTRODUCTION

Anaerobic digestion is a biotechnological process with a promising capabilities for solving some energy and ecological problems in agriculture and agro-industry. In this bioreaction, generally carried out in continuously stirred tank bioreactors, the organic matter is depolluted by microorganisms into biogas (methane and carbon dioxide) and digestate (natural manure) in the absence of oxygen Ahning [2003a,b], Deublein and Steinhauser [2010]. The biogas is an additional energy source and the methane is a greenhouse gas.

Unfortunately this process sometimes is very unstable and needs to be controlled with modern tools. Livestock waste is a complex substrate and its anaerobic degradation consists of a complex series of reactions catalysed by a consortium of different bacteria Gerardi [2003]. Co-digestion of several wastes (manure, sewage sludge and wastes from food processing industry) is another environmentally attractive method for the treatment and recycling of organic wastes. Successful combination of different types of wastes requires the ability to predict the outcome of the process when mixing new wastes. However it is practically impossible to measure on-line the main variables: concentrations of the different populations of microorganisms and/or their

specific growth rates Simeonov [2010], Dochain and Vanrolleghem [2001].

Mathematical modeling represents a very attractive tool for studying this process Deublein and Steinhauser [2010], Gerardi [2003], Simeonov [2010], Dochain and Vanrolleghem [2001], Angelidaki et al. [1999], Batstone et al. [2001], Hill and Barth [1977], Simeonov [1999], Simeonov et al. [2001], however a lot of models are not appropriate for monitoring and control purposes due to their complexity. Relatively simple models of this process, estimation of their parameters, and design of software sensors for the variables which cannot be measured are very important steps for the implementation of sophisticated control algorithms Lubenova et al. [2002], Lopez-Bañuelos et al. [2008]. Continuing works started in Chorukova et al. [2007], Diop and Simeonov [2009], the differential algebraic approach of observation problems is used to obtain new insights in the estimation problems of anaerobic digestion.

Specifically, the concentrations of two different populations of bacteria (acidogenic and methanogenic) and their specific growth rates are estimated on the basis of a 3-stage model and simultaneous measurements of CH<sub>4</sub> and CO<sub>2</sub> in the biogas. The estimation schemes thus obtained have quite interesting features one of which is their freeness of most yield parameters often hard to identify, and the concentration of dry matter in the influent.

The paper is organized as follows. In the next section the pilot bioreactor is presented along with the experiments

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being conducted in. In section 3 the 3-stage model which was validated with the bioreactor is described. The observability analysis and the estimators design are derived in section 4. Section 5 presents illustrative simulations of the estimators are provided. The full experimental validation of these estimators are being prepared for the final version of this paper.

## 2. THE PILOT PLANT

Experimental studies of anaerobic digestion of cattle manure have been performed during the start-up of a 100 m<sup>3</sup> pilot anaerobic plant in mesophilic temperature (34 °C). The scheme of this pilot plant along with its monitoring and control units is shown in Fig. 1.

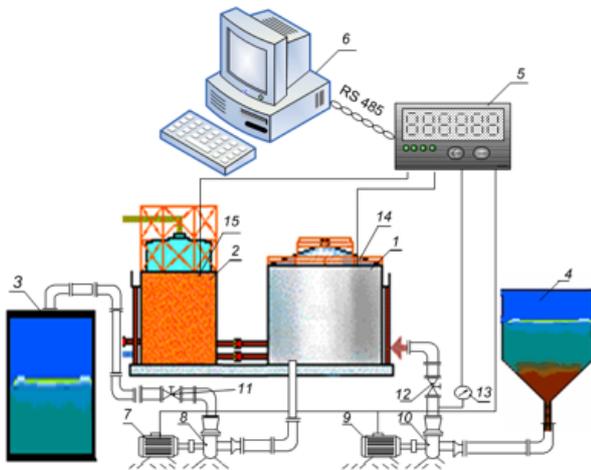


Fig. 1. The pilot plant with its monitoring and control units. Here 1 is the bioreactor, 2 the gasholder, 3 the reservoir for digestate, 4 the vessel for substrate, 5 the controller Bechhoff, 6 the computer, 8 and 10 the two pumps, 7 and 9 the two drives, 11 and 12 the two stop valves, 13, 14 and 15 the temperature sensor, the biogas flow rate and contents of CH<sub>4</sub> and CO<sub>2</sub> sensors in the biogas.

The bioreactor has been started and operated in continuous mode with cattle manure and different values of the dilution rate  $D$  and of the concentration of dry matter in the influent  $S_{in}$ , see Figs 2 and 3.

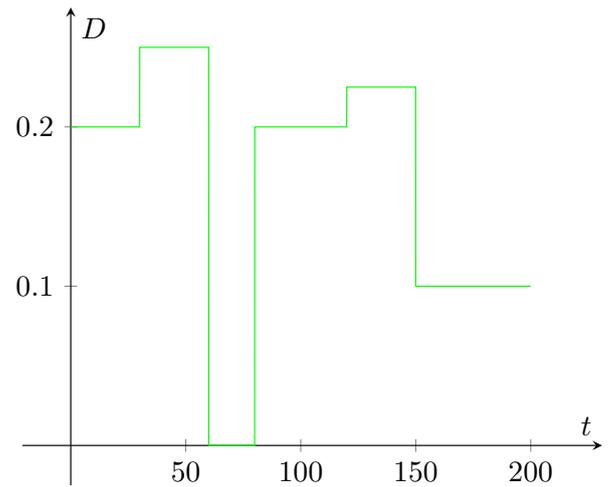


Fig. 2. The dilution rate profile used in experiments.

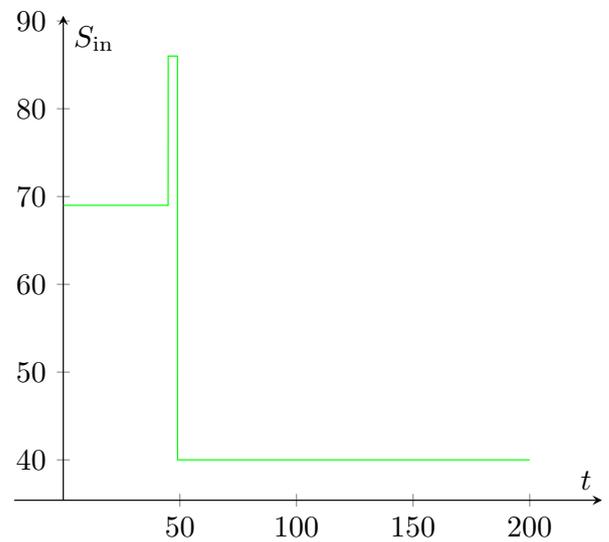


Fig. 3. The concentration of dry matter in the influent

The daily biogas flow-rates per dm<sup>3</sup> of the working volume of the bioreactor are shown in Figs. 4 and 5.

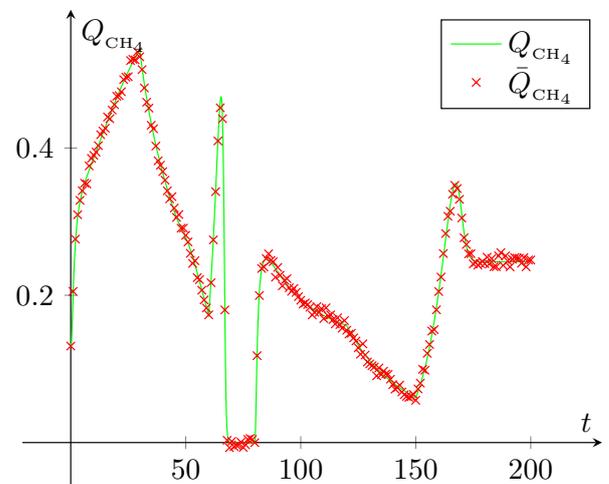


Fig. 4. The methane flow rate

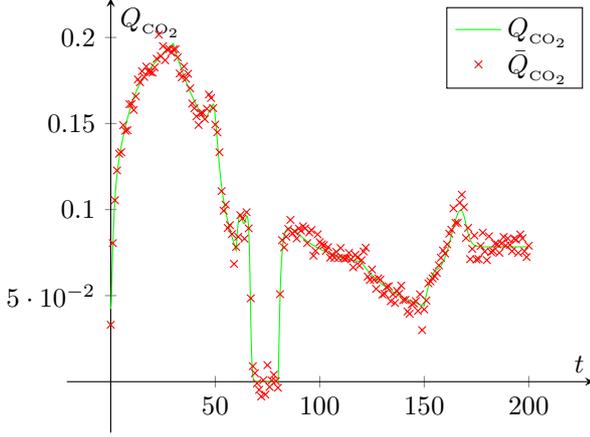


Fig. 5. The carbon dioxide flow rate

### 3. THE PROCESS MODEL

Hill and Barth (in 1977) considered hydrolysis (enzymatic degradation of insoluble organics to soluble organics), acidogenesis (transformation of the soluble organics to acetate) and methanogenesis (transformation of the acetate to methane) (see Fig. 6), developing a model for anaerobic digestion of animal waste as follows:

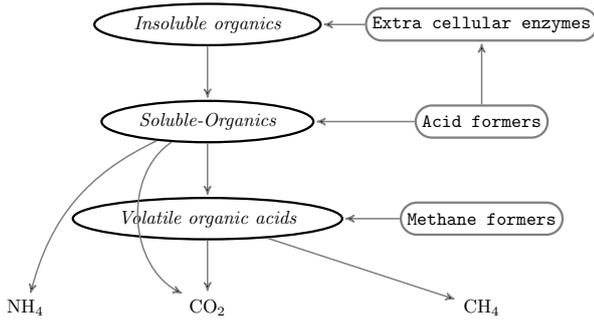


Fig. 6. Flow chart of Hill and Barth (1977) mathematical model

$$\dot{S}_0 = -D S_0 - \beta S_0 X_1 + Y_p D S_{in} \quad (1a)$$

$$\dot{X}_1 = (\mu_1 - k_1 - D) X_1 \quad (1b)$$

$$\dot{S}_1 = -D S_1 + \beta S_0 X_1 - \mu_1 \frac{X_1}{Y_1} \quad (1c)$$

$$\dot{X}_2 = (\mu_2 - k_2 - D) X_2 \quad (1d)$$

$$\dot{S}_2 = -D S_2 + Y_b \mu_1 X_1 - \mu_2 \frac{X_2}{Y_2} \quad (1e)$$

where  $X_1$  and  $X_2$  are the acidogenic (with specific growth rate  $\mu_1$  in  $\text{day}^{-1}$ ) and methanogenic (with specific growth rate  $\mu_2$  in  $\text{day}^{-1}$ ) bacteria concentrations in  $\text{g}/\text{dm}^3 \text{ day}^{-1}$ , respectively.  $S_1$  is the carbohydrates concentration in  $\text{g}/\text{dm}^3$ ,  $S_2$  is the acetate concentration in  $\text{g}/\text{dm}^3$ .

Equation (1a) describes the hydrolysis of cattle manure with concentration  $S_{in}$  resulting in soluble organics with

concentration  $S_0$  ( $\beta$  and  $Y_p$  are coefficients of appropriate dimensions). Equations (1b) and (1c) describe the acidogenic step, equations (1d) and (1e) describe the methanogenic step. In this model  $Y_1$ ,  $Y_2$ , and  $Y_b$  are yield coefficients of appropriate dimensions.

This model has been verified for anaerobic digestion of cattle manure with the addition of various stimulating substances, see Simeonov et al. [2001] for details.

In the present work the biogas is assumed to consist solely of methane and carbon dioxide with models:

$$Q_{\text{CH}_4} = K_{X_2 \text{CH}_4} \mu_2 X_2 \quad (2a)$$

$$Q_{\text{CO}_2} = K_{X_1 \text{CO}_2} \mu_1 X_1 + K_{X_2 \text{CO}_2} \mu_2 X_2 \quad (2b)$$

In all cases the washout of microorganisms is undesirable. That is why changes of the control input  $D$  and the external perturbation  $S_{0i}$  are possible only in some admissible ranges as follows:

$$0 \leq D \leq D_{\text{sup}}, \quad S_{0i}^{\text{min}} \leq S_{0i} \leq S_{0i}^{\text{max}}$$

It has been proved (see Simeonov [1999]) that for this model the static characteristic of the overall biogas flow rate  $Q = Q(D)$  exhibits one single maximum in the previous admissible domain of  $D$ .

### 4. DESIGN OF THE ESTIMATOR

The differential algebraic approach (see Diop [2002]) is used here to analyze the observability of some of the bioreactor variables. For the following 3-stage model of the anaerobic digestion model

$$\begin{cases} \dot{S}_0 = -D S_0 - \beta S_0 X_1 + Y_p D S_{in} \\ \dot{X}_1 = (\mu_1 - k_1 - D) X_1 \\ \dot{S}_1 = -D S_1 + \beta S_0 X_1 - \mu_1 \frac{X_1}{Y_1} \\ \dot{X}_2 = (\mu_2 - k_2 - D) X_2 \\ \dot{S}_2 = -D S_2 + Y_b \mu_1 X_1 - \mu_2 \frac{X_2}{Y_2} \\ Q_{\text{CH}_4} = K_{X_2 \text{CH}_4} \mu_2 X_2 \\ Q_{\text{CO}_2} = K_{X_1 \text{CO}_2} \mu_1 X_1 + K_{X_2 \text{CO}_2} \mu_2 X_2 \end{cases}$$

the analysis of the observability of  $\mu_1$  and  $\mu_2$  with respect to  $D$ ,  $S_{in}$ ,  $Q_{\text{CH}_4}$ ,  $Q_{\text{CO}_2}$ , and all parameters (these are supposed to be *constant* and *known*) yields the following differential polynomials

$$\begin{aligned} & K_{X_2 \text{CO}_2} Q_{\text{CH}_4} \dot{\mu}_1 - K_{X_2 \text{CO}_2} \mu_1 \dot{Q}_{\text{CH}_4} - \\ & K_{X_2 \text{CH}_4} Q_{\text{CO}_2} \dot{\mu}_1 + K_{X_2 \text{CH}_4} \dot{Q}_{\text{CO}_2} \mu_1 - \\ & k_1 K_{X_2 \text{CO}_2} Q_{\text{CH}_4} \mu_1 + K_{X_2 \text{CO}_2} Q_{\text{CH}_4} \mu_1^2 - \\ & K_{X_2 \text{CH}_4} Q_{\text{CO}_2} \mu_1^2 - K_{X_2 \text{CO}_2} D Q_{\text{CH}_4} \mu_1 + \\ & k_1 K_{X_2 \text{CH}_4} Q_{\text{CO}_2} \mu_1 + \\ & K_{X_2 \text{CH}_4} D Q_{\text{CO}_2} \mu_1 \end{aligned} \quad (3)$$

$$\begin{aligned} & -k_2 \mu_2 Q_{\text{CH}_4} + \dot{\mu}_2 Q_{\text{CH}_4} + \mu_2^2 Q_{\text{CH}_4} - \\ & \mu_2 \dot{Q}_{\text{CH}_4} - \mu_2 Q_{\text{CH}_4} D \end{aligned} \quad (4)$$

$$\frac{K_{X_1CO_2}K_{X_2CH_4}\mu_1X_1 + K_{X_2CO_2}Q_{CH_4} - K_{X_2CH_4}Q_{CO_2}}{K_{X_2CH_4}Q_{CO_2}} \quad (5)$$

$$-K_{X_2CH_4}\mu_2X_2 + Q_{CH_4} \quad (6)$$

$$\begin{aligned} & -K_{X_2CO_2}\beta S_0Q_{CH_4} - K_{X_1CO_2}K_{X_2CH_4}Y_p\mu_1S_{in}D + \\ & K_{X_1CO_2}K_{X_2CH_4}\mu_1\dot{S}_0 + K_{X_1CO_2}K_{X_2CH_4}\mu_1S_0D + \\ & K_{X_2CH_4}\beta S_0Q_{CO_2} \end{aligned} \quad (7)$$

$$\begin{aligned} & K_{X_2CO_2}Y_1\beta S_0Q_{CH_4} - K_{X_2CO_2}\mu_1Q_{CH_4} + \\ & K_{X_1CO_2}K_{X_2CH_4}Y_1\mu_1\dot{S}_1 + \\ & K_{X_1CO_2}K_{X_2CH_4}Y_1\mu_1S_1D - K_{X_2CH_4}Y_1\beta S_0Q_{CO_2} + \\ & K_{X_2CH_4}\mu_1Q_{CO_2} \end{aligned} \quad (8)$$

$$\begin{aligned} & K_{X_2CO_2}Y_bY_2Q_{CH_4} + K_{X_1CO_2}K_{X_2CH_4}Y_2\dot{S}_2 + \\ & K_{X_1CO_2}K_{X_2CH_4}Y_2S_2D + K_{X_1CO_2}Q_{CH_4} - \\ & K_{X_2CH_4}Y_bY_2Q_{CO_2} \end{aligned} \quad (9)$$

The reader may refer to Diop [2002] and Chorukova et al. [2007] for more details and references on the differential algebraic decision methods which provide this observability test.

Rewritten, the first two differential polynomials (3 and 4) yield the following differential equations

$$\begin{aligned} & (K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4})\dot{\mu}_1 - \\ & (K_{X_2CH_4}\dot{Q}_{CO_2} - K_{X_2CO_2}\dot{Q}_{CH_4})\mu_1 - \\ & (D + k_1)(K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4})\mu_1 + \\ & (K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4})\mu_1^2 = 0 \end{aligned} \quad (10)$$

$$\begin{aligned} & Q_{CH_4}\dot{\mu}_2 - \dot{Q}_{CH_4}\mu_2 - (D + k_2)Q_{CH_4}\mu_2 + \\ & Q_{CH_4}\mu_2^2 = 0 \end{aligned} \quad (11)$$

In any time interval where  $\mu_1$  is identically zero equation (10) reduces to the trivial one  $0 = 0$ . The same is true for  $\mu_2$  and equation (11), respectively. In what follows it is supposed that there is at least one time interval where none of  $\mu_i$  ( $i = 1$  or  $2$ ) is not identically zero, and the differential equation (10) (respectively, (11)) is considered to be defined in such a time interval. Dividing equation (10) by  $\mu_1^2$  and equation (11) by  $\mu_2^2$  the previous differential equations become

$$\begin{aligned} & \left( \frac{K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4}}{\mu_1} \right)^{\bullet} = \\ & -(D + k_1) \frac{K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4}}{K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4}} + \end{aligned} \quad (12)$$

$$\left( \frac{Q_{CH_4}}{\mu_2} \right)^{\bullet} = -(D + k_2) \frac{Q_{CH_4}}{\mu_2} + Q_{CH_4} \quad (13)$$

which, in turn, may be rewritten as follows

$$\begin{cases} q_{CO_2} = K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4} \\ \dot{z}_1 = -(D + k_1)z_1 + q_{CO_2} \\ \mu_1 = \frac{q_{CO_2}}{z_1} \end{cases} \quad (14)$$

$$\begin{cases} \dot{z}_2 = -(D + k_2)z_2 + Q_{CH_4} \\ \mu_2 = \frac{Q_{CH_4}}{z_2} \end{cases} \quad (15)$$

*Remark 1.* The quantity  $q_{CO_2}$  is nonnegative since, given equations (2), it evaluates to

$$q_{CO_2} = K_{X_1CO_2}K_{X_2CH_4}\mu_1X_1.$$

The previous two systems of differential equations provide dynamic estimation schemes for the specific growth rates and biomass concentrations as stated in the following

*Theorem 2.* Assuming the inputs  $D$  and  $S_{in}$  free of  $z_i$  ( $i = 1$  or  $2$ ) the previous differential equation (14) or (15) is readily a dynamic estimator of quantities of interest:

$$\begin{cases} q_{CO_2} = K_{X_2CH_4}Q_{CO_2} - K_{X_2CO_2}Q_{CH_4} \\ \dot{z}_1 = -(D + k_1)z_1 + q_{CO_2} \\ \hat{\mu}_1 = \frac{q_{CO_2}}{z_1} \\ \hat{X}_1 = \frac{z_1}{K_{X_1CO_2}K_{X_2CH_4}} \end{cases} \quad (16)$$

$$\begin{cases} \dot{z}_2 = -(D + k_2)z_2 + Q_{CH_4} \\ \hat{\mu}_2 = \frac{Q_{CH_4}}{z_2} \\ \hat{X}_2 = \frac{z_2}{K_{X_2CH_4}} \end{cases} \quad (17)$$

Since  $\mu_i$  ( $i = 1$  or  $2$ ) is assumed unknown the initial condition of  $z_i$  will be set up with some error, but, in every time interval  $[r, s]$  where the quantity  $D + k_i$  ( $i = 1$  or  $2$ ) is positive, the estimation error  $\tilde{z}_i = z_i - \hat{z}_i$  which is due to the mis-initialization of  $z_i$  will tend to zero as follows

$$\tilde{z}_i(t) = \tilde{z}_i(r) \exp\left(-\int_r^t (D(\tau) + k_i)d\tau\right)$$

when  $t$  tends to  $s$ . Here  $\tilde{z}_i(r)$  is the error between the true value  $z_i$  and its initialization  $\hat{z}_i$ . In other words,  $z_i$  converges exponentially to  $z_i$  whenever  $D + k_i$  is positive.

The speed of convergence of these estimators is fixed by the quantity  $D + k_i$  ( $i = 1$  or  $2$ ). Specifically, the following shows how long piecewise constant changes in  $D$  should be scheduled in order to ease the estimation convergence.

*Corollary 3.* If, in addition to the conditions of the above theorem, the input  $D$  is constant in the time interval  $[r, s]$  then the error  $\tilde{z}_i(s)$  is reduced by 95% with respect to  $\tilde{z}_i(r)$  (that is,  $\tilde{z}_i(s)/\tilde{z}_i(r) = 0.05$ ) whenever

$$s - r \approx \frac{3}{D + k_i}.$$

*Remark 4.* In practice not only there is an initialization error for  $z_i$  ( $i = 1$  or  $2$ ) but there are also uncertainties on measurements  $Q_{\text{CH}_4}$  and  $Q_{\text{CO}_2}$ . The estimation errors are thus given by

$$\tilde{z}_1(t) = \tilde{z}_1(r) \exp\left(-\int_r^t (D(\tau) + k_1)d\tau\right) + \int_r^t \tilde{q}_{\text{CO}_2}(\tau) \exp\left(-\int_r^\tau (D(\sigma) + k_1)d\sigma\right) d\tau$$

and

$$\tilde{z}_2(t) = \tilde{z}_2(r) \exp\left(-\int_r^t (D(\tau) + k_2)d\tau\right) + \int_r^t \tilde{Q}_{\text{CH}_4}(\tau) \exp\left(-\int_r^\tau (D(\sigma) + k_2)d\sigma\right) d\tau$$

where  $\tilde{q}_{\text{CO}_2} = q_{\text{CO}_2} - \bar{q}_{\text{CO}_2}$ ,  $Q_{\text{CH}_4} = Q_{\text{CH}_4} - \bar{Q}_{\text{CH}_4}$  with  $\bar{Q}_{\text{CH}_4}$  and  $\bar{Q}_{\text{CO}_2}$  are the respective measured values of  $Q_{\text{CH}_4}$  and  $Q_{\text{CO}_2}$ , and  $\bar{q}_{\text{CO}_2} = K_{\text{X}_2\text{CH}_4}\bar{Q}_{\text{CO}_2} - K_{\text{X}_2\text{CO}_2}\bar{Q}_{\text{CH}_4}$ .

## 5. SIMULATION ILLUSTRATIONS

The following figures illustrate the performance of the estimators. The online data which feed the estimators are as shown in Figs. 2, 4, and 5. They are daily samples of the corresponding continuous time variables. The measurements noise have been simulated as a normal random variable with variance 0.005.

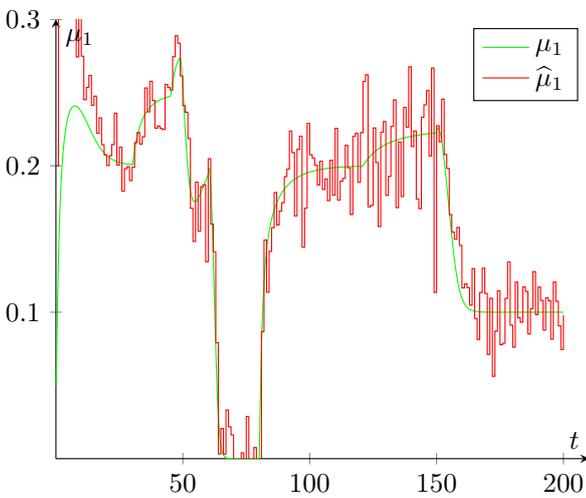


Fig. 7. The simulated noise in the methane flow rate is directly visible on  $\mu_1$  according to equations (16)

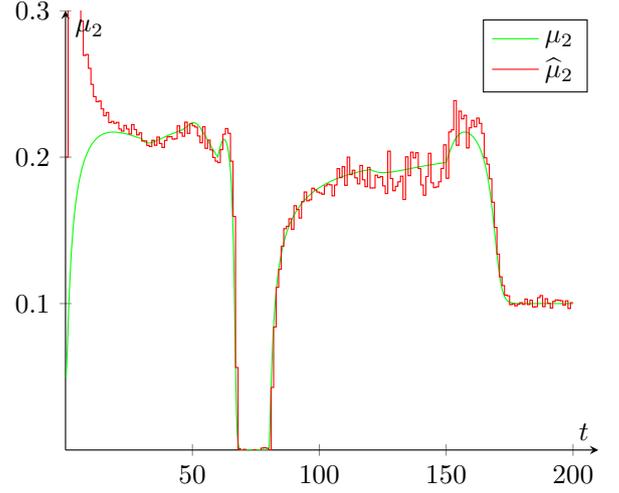


Fig. 8. The less noise (compared to  $\mu_1$ ) which is apparent in  $\mu_2$  is due to the value of  $q_{\text{CO}_2}$  as shown in equation (16).

As expected from equations (16) and (17) the noise has been filtered out of  $X_1$  and  $X_2$  thanks to the expressions of the latter variables in  $z_1$  and  $z_2$ .

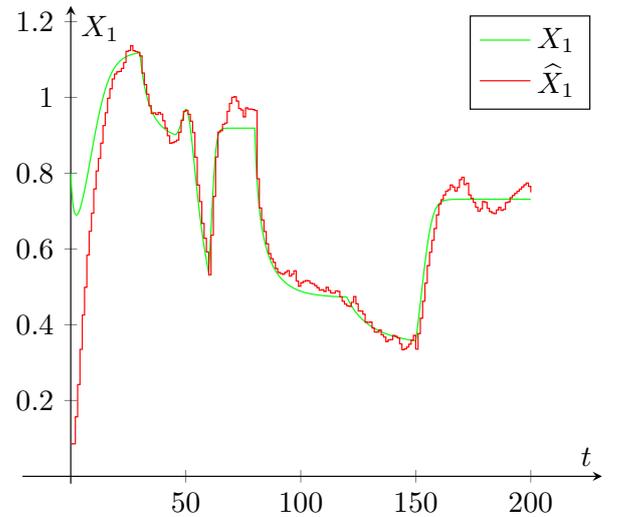


Fig. 9. When the piecewise constants in  $D$  last sufficiently long the convergence (as indicated in Corollary 3) of  $X_1$  is quite guaranteed.

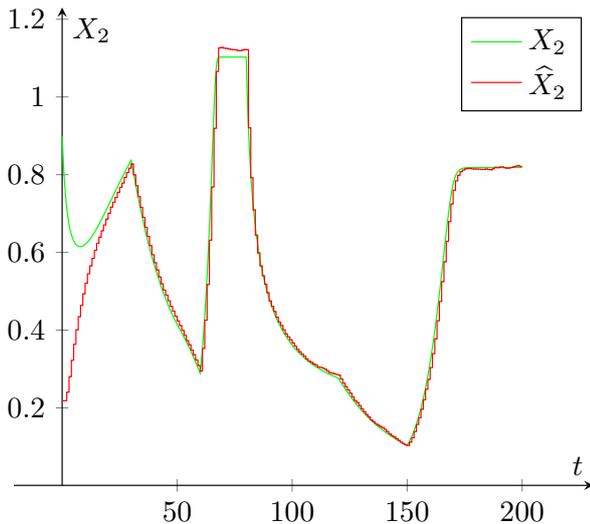


Fig. 10. As stated in Theorem 2, in time intervals where  $D + k_2$  is identically zero (here  $D + k_2 = 0$  between the 60th and 80th days) the exponential convergence is lost.

## 6. CONCLUSION

Experimental studies of the anaerobic digestion of cattle dung in a pilot continuously stirred tank bioreactor are being done. Estimators of concentrations of two different populations of microorganisms (acidogenic and methanogenic) and their specific growth rates have been designed on the basis of a 3-stage model and simultaneous measurements of  $\text{CH}_4$  and  $\text{CO}_2$  in the biogas. While these results are being experimentally verified quite realistic simulations are presented showing the performance of the proposed estimators. Before these estimation schemes are used in control strategies for the pilot bioreactor their robustness with respect to the few parameters they involve have to be ascertained since, as is well-known, anaerobic digestion is a complex process with parameters hard to identify accurately.

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