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

S. Diop[1] and I. Simeonov[2]

***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 currently being confronted to experimental data from a $100\,\mathrm{m}^3$ pilot bioreactor fed with cattle dung. Realistic simulations are presented in this paper as illustrations of the estimator performance.**

I. 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 [1, 2, 6]. 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 catalyzed by a consortium of different bacteria [10]. 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 [9, 16].

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Mathematical modeling represents a very attractive tool for studying this process [3, 4, 6, 9–11, 15–17], 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 [13, 14]. Continuing works started in [5, 8], 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_4 and CO_2 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 being conducted in it. 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.

II. The pilot plant

Experimental studies of anaerobic digestion of cattle manure have been performed during the start-up of a $100\,\mathrm{m}^3$ pilot anaerobic plant in mesophillic temperature ($34\,^\circ\mathrm{C}$). The scheme of this pilot plant along with its monitoring and control units is shown in Fig. 1.

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.

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

III. The process model

Hill and Barth (in 1977) considered hydrolysis (enzymatic degradation of insoluble organics to soluble organics), acidogenesis (transformation of the soluble organics

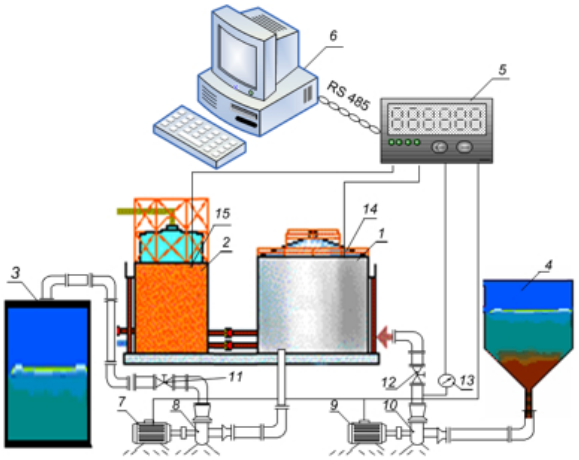


Fig. 1: The pilot plant with its monitoring and control units. Here 1 is the bioreactor, 2 the gasholder, 3 the reservoir for digestate, 4 the vessel for substrate, 5 the controller Bechhoff, 6 the computer, 8 and 10 the two pumps, 7 and 9 the two drives, 11 and 12 the two stop valves, 13, 14 and 15 the temperature sensor, the biogas flow rate and contents of CH_4 and CO_2 sensors in the biogas.

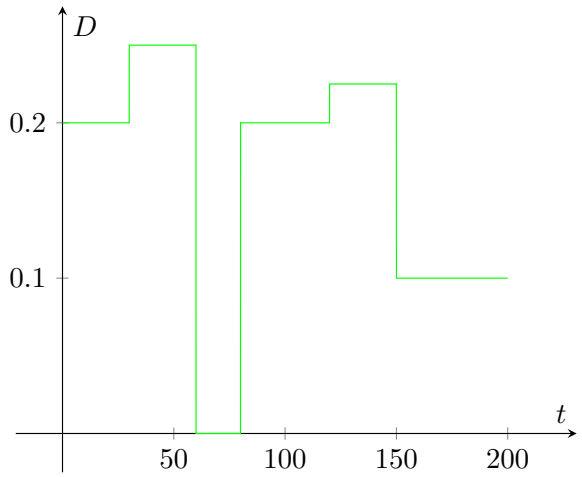


Fig. 2: The dilution rate profile used in experiments.

to acetate) and methanogenesis (transformation of the acetate to methane) (see Fig. 6), developing a model for anaerobic digestion of animal waste as follows:

$$\dot{S}_0 = -D\,S_0 - \beta S_0 X_1 + Y_\mathrm{p} D\,S_\mathrm{in} \tag{1a}$$

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

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

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

$$\dot{S}_2 = -D\,S_2 + Y_\mathrm{b}\mu_1 X_1 - \mu_2 \frac{X_2}{Y_2} \tag{1e}$$

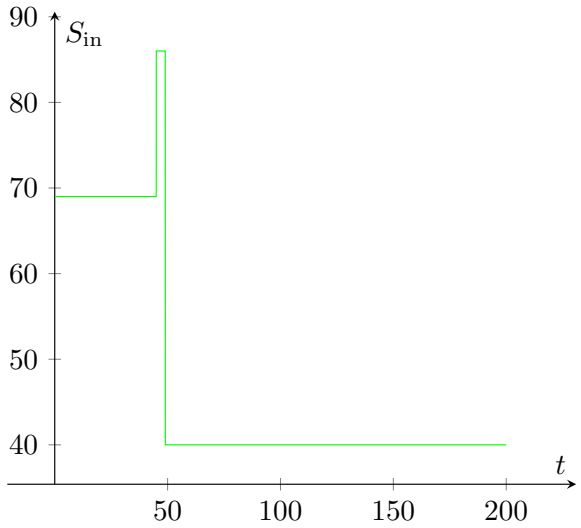


Fig. 3: The concentration of dry matter in the influent

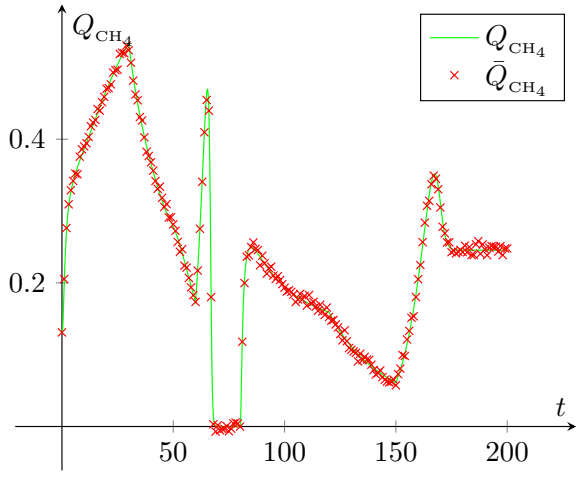


Fig. 4: The methane flow rate

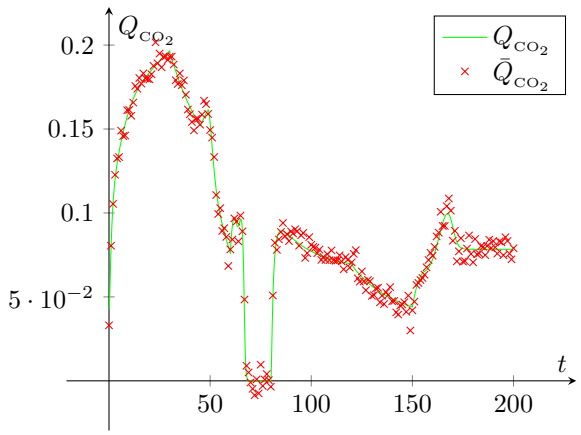


Fig. 5: The carbon dioxide flow rate

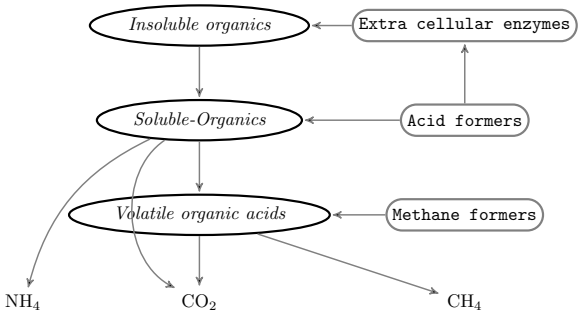


Fig. 6: Flow chart of Hill and Barth (1977) mathematical model

where X_1 and X_2 are the acidogenic (with specific growth rate μ_1 in day^{-1}) and methanogenic (with specific growth rate μ_2 in day^{-1}) bacteria concentrations in g/dm^3 day^{-1}, respectively. S_1 is the carbohydrates concentration in g/dm^3, S_2 is the acetate concentration in g/dm^3.

Equation (1a) describes the hydrolysis of cattle manure with concentration S_{in} resulting in soluble organics with concentration S_0 (β and Y_{p} are coefficients of appropriate dimensions). Equations (1b) and (1c) describe the acidogenyc step, equations (1d) and (1e) describe the methanogenyc 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 [17] for details.

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

$$Q_{\text{CH}_4} = K_{\text{X}_2\text{CH}_4}\mu_2 X_2 \tag{2a}$$

$$Q_{\text{CO}_2} = K_{\text{X}_1\text{CO}_2}\mu_1 X_1 + K_{\text{X}_2\text{CO}_2}\mu_2 X_2 \tag{2b}$$

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

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

It has been proved (see [15]) 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.

IV. Design of the estimator

The differential algebraic approach (see [7]) is used here to analyze the observability of some of the bioreactor variables. For the following 3-stage model of the anaerobic digestion model

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

the analysis of the observability of μ_1 and μ_2 with respect to D, S_{in}, Q_{CH_4}, Q_{CO_2}, and all parameters (these are supposed to be *constant* and *known*) yields the following differential polynomials

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

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

$$\begin{aligned} &K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4}\mu_1 X_1 + K_{\text{X}_2\text{CO}_2} Q_{\text{CH}_4} - \\ &K_{\text{X}_2\text{CH}_4} Q_{\text{CO}_2} \end{aligned} \tag{5}$$

$$-K_{\text{X}_2\text{CH}_4}\mu_2 X_2 + Q_{\text{CH}_4} \tag{6}$$

$$\begin{aligned} &-K_{\text{X}_2\text{CO}_2}\beta S_0 Q_{\text{CH}_4} - K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4} Y_{\text{p}}\mu_1 S_{\text{in}} D + \\ &K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4}\mu_1\dot{S}_0 + K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4}\mu_1 S_0 D + \\ &K_{\text{X}_2\text{CH}_4}\beta S_0 Q_{\text{CO}_2} \end{aligned} \tag{7}$$

$$\begin{aligned} &K_{\text{X}_2\text{CO}_2} Y_1\beta S_0 Q_{\text{CH}_4} - K_{\text{X}_2\text{CO}_2}\mu_1 Q_{\text{CH}_4} + \\ &K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4} Y_1\mu_1\dot{S}_1 + \\ &K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4} Y_1\mu_1 S_1 D - K_{\text{X}_2\text{CH}_4} Y_1\beta S_0 Q_{\text{CO}_2} + \\ &K_{\text{X}_2\text{CH}_4}\mu_1 Q_{\text{CO}_2} \end{aligned} \tag{8}$$

$$\begin{aligned} &K_{\text{X}_2\text{CO}_2} Y_{\text{b}} Y_2 Q_{\text{CH}_4} + K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4} Y_2\dot{S}_2 + \\ &K_{\text{X}_1\text{CO}_2} K_{\text{X}_2\text{CH}_4} Y_2 S_2 D + K_{\text{X}_1\text{CO}_2} Q_{\text{CH}_4} - \\ &K_{\text{X}_2\text{CH}_4} Y_{\text{b}} Y_2 Q_{\text{CO}_2} \end{aligned} \tag{9}$$

The reader may refer to [7] and [5] 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

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

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

In any time interval where μ_1 is identically zero equation (10) reduces to the trivial one $0=0$. The same is true for μ_2 and equation (11), respectively. In what follows *it is supposed that there is at least one time interval where none of μ_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 μ_1^2 and equation (11) by μ_2^2 the previous differential equations become

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

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

which, in turn, may be rewritten as follows

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

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

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

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

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:

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

$$\begin{cases}\dot{z}_2=-(D+k_2)z_2+Q_{\mathrm{CH_4}}\\\widehat{\mu}_2=\dfrac{Q_{\mathrm{CH_4}}}{z_2}\\\widehat{X}_2=\dfrac{z_2}{K_{\mathrm{X_2CH_4}}}\end{cases}\tag{17}$$

Since μ_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 $\widetilde{z}_i=z_i-\widehat{z}_i$ which is due to the mis-initialization of z_i will tend to zero as follows

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

when t tends to s. Here $\widetilde{z}_i(r)$ is the error between the true value z_i and its initialization $\widehat{z}_i$. 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 $\widetilde{z}_i(s)$ is reduced by 95% with respect to $\widetilde{z}_i(r)$ (that is, $\widetilde{z}_i(s)/\widetilde{z}_i(r)=0.05$) 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 $Q_{\mathrm{CH_4}}$ and $Q_{\mathrm{CO_2}}$. The estimation errors are thus given by

$$\begin{aligned}\widetilde{z}_1(t)\ &=\ \widetilde{z}_1(r)\ \exp\left(-\int_r^t(D(\tau)+k_1)\mathrm{d}\tau\right)+\\&\int_r^t\widetilde{q}_{\mathrm{CO_2}}(\tau)\exp\left(-\int_\tau^t(D(\sigma)+k_1)\mathrm{d}\sigma\right)\mathrm{d}\tau\end{aligned}$$

and

$$\begin{aligned}\widetilde{z}_2(t)\ &=\ \widetilde{z}_2(r)\ \exp\left(-\int_r^t(D(\tau)+k_2)\mathrm{d}\tau\right)+\\&\int_r^t\widetilde{Q}_{\mathrm{CH_4}}(\tau)\exp\left(-\int_\tau^t(D(\sigma)+k_2)\mathrm{d}\sigma\right)\mathrm{d}\tau\end{aligned}$$

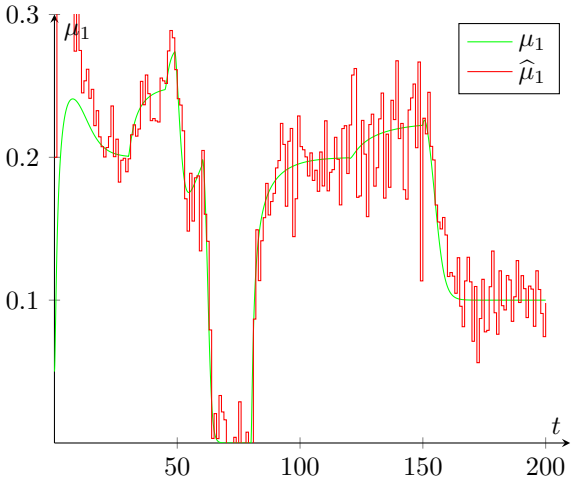


Fig. 7: The simulated noise in the methane flow rate is directly visible on μ_1 according to equations (16)

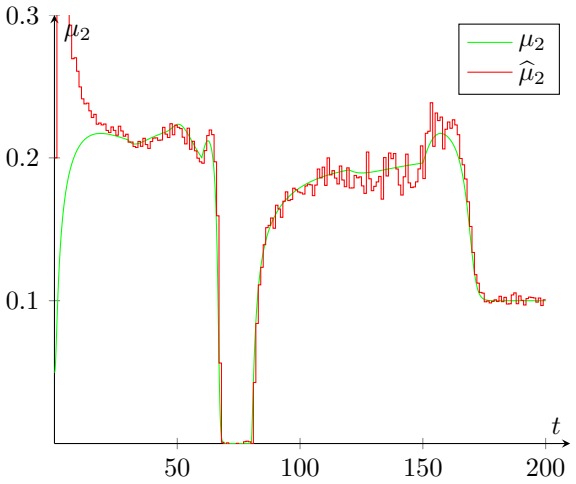


Fig. 8: The less noise (compared to μ_1) which is apparent in μ_2 is due to the value of q_{CO_2} as shown in equation (16).

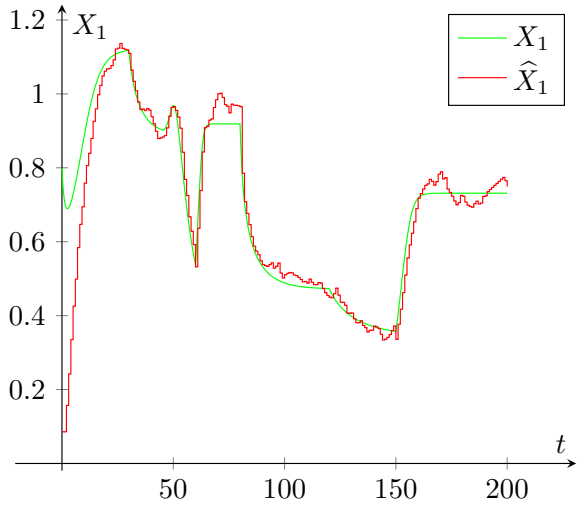


Fig. 9: When the piecewise constants in D last sufficiently long the convergence (as indicated in Corollary 3) of X_1 is quite guaranteed.

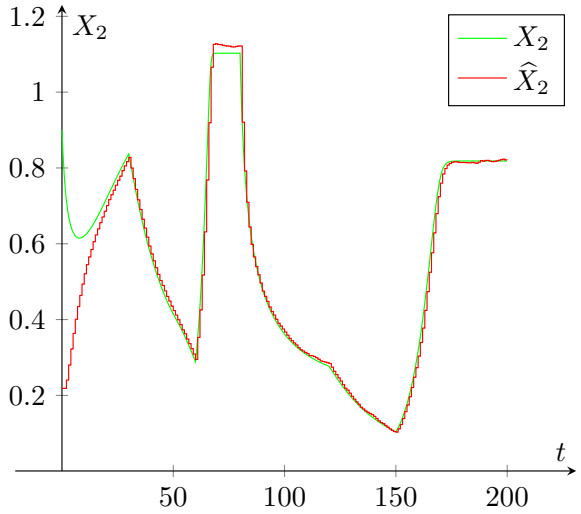


Fig. 10: As stated in Theorem 2, in time intervals where $D + k_2$ is identically zero (here $D + k_2 = 0$ between the 60th and 80th days) the exponential convergence is lost.

where $\widetilde{q}_{\mathrm{CO}_2} = q_{\mathrm{CO}_2} - \bar{q}_{\mathrm{CO}_2}$, $Q_{\mathrm{CH}_4} = Q_{\mathrm{CH}_4} - \bar{Q}_{\mathrm{CH}_4}$ with $\bar{Q}_{\mathrm{CH}_4}$ and $\bar{Q}_{\mathrm{CO}_2}$ are the respective measured values of Q_{CH_4} and Q_{CO_2}, and $\bar{q}_{\mathrm{CO}_2} = K_{\mathrm{X_2CH_4}}\bar{Q}_{\mathrm{CO}_2} - K_{\mathrm{X_2CO_2}}\bar{Q}_{\mathrm{CH}_4}$.

V. 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.
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 andz_2.

VI. 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 CH_4 and 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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