

V. BIOAUTOMATICS AND BIOINFORMATICS

MODELING AND SOFTWARE SENSORS DESIGN FOR ANAEROBIC DIGESTION PROCESS

E. Chorukova, S. Diop, I. Simeonov, S. Tebbani

Abstract. Anaerobic digestion is an effective biotechnological process for treatment of different agricultural, municipal and industrial wastes. Use of mathematical models is a powerful tool for investigations and optimisation of the anaerobic digestion processes and for software sensors design as well. In this paper a new version, concerning the gas phase modelling of a simple mathematical model of the anaerobic digestion was developed and verified experimentally. The parameter identification was based on a set of 150 days of dynamical experiments in a laboratory bioreactor. Two step identification procedure to estimate 3 model parameters is presented. The results of 15 days of experiment in a pilot-scale bioreactor were then used to validate the model.

On the base of the modified simple mathematical model of the AD software sensors using the differential algebraic approach were designed and studied by simulations.

Keywords: anaerobic digestion, wasted fruits and vegetables, mathematical model, specific growth rate estimation, control systems observability theory.

1. INTRODUCTION

Anaerobic digestion (AD) is an effective biotechnological process for treatment of different agricultural, municipal and industrial wastes [1,2]. It combines environmental depollution (ecological aspect) with production of renewable energy – biogas, the main component of which is methane (energetical aspect). However, AD is a very unstable process in regard to biogas reactors operation due to the complicated interactions between different microbial species, as well as to the complex transformations of organic matter affected by a variety of environmental factors [3]. In this context, the use of mathematical models is a powerful tool for investigations, software sensors design, optimisation and control of the AD [4,...,9]. ADM1 [7] is the most complex and powerful AD model. However, such types of models are very complex for practical use.

In [9] a quite realistic fruits and vegetables AD model was developed and validated with laboratory and pilot scale experimental data. However the gas-phase modeling was too complicated for software sensors design using differential algebraic approach (enormous expressions were obtained).

The aim of this study is to modify and verify experimentally the mathematical model of the AD from [9] in order to develop realistic software sensors using the differential algebraic approach.

2. EXPERIMENTAL STUDIES

The experiments were carried out in a 100-L pilot scale anaerobic BR with a working volume of

80 L in mesophilic temperature (34 ± 0.5 °C) [10]. The bioreactor was operated in semi-continuous mode. The substrate was stored in plastic can of 25 L placed in the influent line of the BR. The digestate taken out of it during semi-continuous operation (feeding one to 24 times daily) is stored in plastic can of 50 L in the next-door auxiliary service premises of the biogas plant.

A biogas outlet from the upper bioreactor flange leads off the biogas to a 200 L metal gasholder (GH) operating on the water displacement principle (the inner vessel, placed in vessel with water, is displaced vertically by the biogas). Daily biogas production was measured by the water displacement technique (graduated gasholder). The biogas flow rate was measured through transformation of the linear shift of the inlet vessel of the GH into normalized electrical signal (sensor developed by our team). The biogas composition was measured with infrared sensors of MSR.

pH in the bioreactors have been measured daily in the effluent with laboratory pH-meter. Samples for pH measurements and biochemical analyses were taken from the effluent of the bioreactor (digestate). Corrections of pH were done (if necessary) with additions of 2 N NaOH in the influent.

Experimental studies of AD with the same mixture of WFV with step change of the dilution rate from 0.025 to 0.0125 and for constant concentration of the total solids in the influent (TS = 70 g/dm³) were performed with the pilot anaerobic plant at mesophilic temperature (34 °C).

3. THE AD MODEL

Generally the AD processes can be divided in four main stages:

- hydrolysis of undissolved high-molecular weight compounds (proteins, sugars, fats) to soluble low-molecular weight compounds (monosugars, aminoacids, long-chain fatty acids, glycerol);

- acidogenesis – fermentation of low-molecular weight compounds from the previous stage to VFA (propionate, butyrate, acetate), hydrogen and carbon dioxide;

- acetogenesis – transformation of VFA to acetate, hydrogen and carbon dioxide;

- methanogenesis mediated by acetoclastic methanogens (converting acetate to methane and carbon dioxide) and hydrogenotrophic methanogens (producing methane from hydrogen and carbon dioxide).

Studying the process of AD of WFV we supposed that the stage of acetogenesis is not so important. In this case the three-stage biochemical scheme [17], describing hydrolysis, acidogenesis and methanogenesis, was adopted.

3.1. Structure of the model

Liquid phase

On the basis of the above-presented experimental studies and according to the relatively simple three-stage biochemical scheme of the AD, the following set of five ODE is adopted for the structure of the model in our case [9]:

$$\frac{dS_0}{dt} = -DS_0 - \beta X_1 S_0 + DY_p S_{in} \quad (1a)$$

$$\frac{dX_1}{dt} = \mu_1 X_1 - DX_1 \quad (1b)$$

$$\frac{dS_1}{dt} = -DS_1 + \beta X_1 S_0 - \frac{1}{Y_1} \mu_1 X_1 \quad (1c)$$

$$\frac{dX_2}{dt} = \mu_2 X_2 - DX_2 \quad (1d)$$

$$\frac{dS_2}{dt} = -DS_2 + Y_b \mu_1 X_1 - \frac{1}{Y_2} \mu_2 X_2 \quad (1e)$$

in which the bacterial growth is of Monod type.

Gas phase modelling

The model presented in [9] was further studied and simplified mainly in the gas phase modelling as follows:

$$\frac{dCO_2}{dt} = -DCO_2 - k_{La}(CO_2 - K_H P_c) + K_{X_1CO_2} \mu_1 X_1 + K_{X_2CO_2} \mu_2 X_2 \quad (1f)$$

$$Q_{CH_4} = K_{X_2CH_4} \mu_2 X_2 \quad (1g)$$

$$Q_{CO_2} = k_{La}(CO_2 - K_H P_c) \quad (1h)$$

$$P_c = \frac{\phi - \sqrt{\phi^2 - 4K_H P_T CO_2}}{2K_H} \quad (1i)$$

$$\phi = CO_2 + K_H P_T + \frac{K_{X_2CH_4}}{k_{La}} \mu_2 X_2$$

where the nomenclature is given in Table 1.

The model is a mass balance one which captures the first stage in anaerobic digestion, namely the hydrolysis, through equation 1a, the acidogenesis stage in equations 1b and 1c and the methanogenesis stage in equations 1d and 1e. The carbone dioxyde is the only component of the biogas which is solvable in the liquid in significant quantity; its concentration in the biogas will be measured by specific gas flow rate devices, and its dissolved part is modeled by equation 1f. There are available sensors for the dissolved carbone dioxyde but their use in bioreactors such as the ones considered here is not recommended due to thickness of the liquid.

3.2. Parameters estimation

We postulated that kinetic and yield coefficients of the mass balance model (Eqs. 1a-1e) are known and we adopted their values from [9]: $\beta = 3, Y_p = 0.14, Y_b = 5, Y_1 = 0.15, Y_2 = 0.24$.

The mass balance model (1) has been complemented by Monod models of specific growth rates:

$$\mu_1 = \frac{\mu_{1max} S_1}{K_{s1} + S_1}$$

$$\mu_2 = \frac{\mu_{2max} S_1}{K_{s2} + S_2}$$

with the coefficients adopted from [9]: $\mu_{1max} = 0.4, K_{s1} = 4.2, \mu_{2max} = 0.25, K_{s2} = 0.42$.

We supposed that only the 5 coefficients ($k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$) of Eqs. 1f-1i, describing the gas phase, are unknown. P_T, k_{La} and K_H for the anaerobic digestion of organic waste we

took from the literature [5]: $P_T = 1, k_{La} = 200, K_H = 0.03$.

For estimation of the rest 3 unknown coefficients nonlinear constrained optimization

method from the “Optimisation toolbox” for MATLAB with gradient method (Sequential quadratic programming) was used.

Table 1: Nomenclature

D	dilution rate [d^{-1}]
S_0, S_{in}	organic substrate concentration [g/dm^3]
X_1	acidogenic bacteria concentration [g/dm^3]
S_1	glucose substrate concentration [g/dm^3]
μ_1	specific growth rate of acidogenic bacteria [d^{-1}]
X_2	methanogenic bacteria concentration [g/dm^3]
S_2	volatile fatty acids concentration [g/dm^3]
μ_2	specific growth rate of methanogenic bacteria [d^{-1}]
Q_{CO_2}	CO_2 flow rate [dm^3/d]
Q_{CH_4}	methane flow rate [dm^3/d]
CO_2	carbon dioxide concentration in the liquid phase [g/dm^3]
CO_2^*	equilibrium value of CO_2 [g/dm^3]
P_c	carbon dioxide partial pressure in the gas phase [atm]
P_T	total pressure [atm]
K_H	Henry's constant [g/dm^3 per atm]
k_{La}	liquid-gas transfer constant [d^{-1}]
$\beta, Y_p, Y_b, Y_1, Y_2$	yield coefficients of appropriate dimensions
$K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$	yield coefficients for carbon dioxide and methane

The procedure finds the minimum of a constrained nonlinear multivariable function (criterion). The following criteria for minimisation were adopted:

$$I_1 = \sum (Q_{CH_4}^{exp} - Q_{CH_4}^{mod el})^2 = \varepsilon_1^2 \rightarrow \min \quad (2a)$$

$$I_2 = \sum (Q_{CO_2}^{exp} - Q_{CO_2}^{mod el})^2 = \varepsilon_2^2 \rightarrow \min \quad (2b)$$

Analysing the experimental data and two steps estimation procedure has been adopted:

- At the first step the unknown methane yield coefficient $K_{X_2CH_4}$ was estimated with experimental data for the specific methane flow-rate $Q_{spCH_4}^{exp}$ calculated from the laboratory-scale data for one step change of the input D (from $D = 0.02$ to $D = 0.04$) and minimization of the criterion (2a). The estimation was made starting from different initial value of the coefficient in the admissible range (0.01 – 40.0). Regardless of the initial value of

the coefficient $K_{X_2CH_4}$, it retains its value of 18.97 (Table 2).

- At the second step we estimate the unknown carbon dioxide yield coefficients $K_{X_1CO_2}$ and $K_{X_2CO_2}$, with laboratory-scale experimental data for the specific carbon dioxide flow-rate $Q_{spCO_2}^{exp}$ for two step change of the input D (from $D = 0.02$ to $D = 0.04$ and from $D = 0.04$ to $D = 0.06$) and minimization of the criterion (2b). The estimation was made starting from different initial value of

Table 2.

Experiment	$K_{X_2CH_4}$	Criterion	$K_{X_2CH_4}$ init. cond.
1	18.97	607.3	0.01
2	18.97	607.3	20
3	18.97	607.3	40

these coefficients in their admissible ranges (0.01 – 40.0). The results for estimation of the coefficients $K_{X_1CO_2}$ and $K_{X_2CO_2}$ are shown in the Table 3.

The conclusion is that all coefficients have unique values which are as follows:

$K_{X_2CH_4} = 18.97$, $K_{X_1CO_2} = 0.1$ and $K_{X_2CO_2} = 10.73$.

Experimental data and data from computer simulation of the model with the obtained values of the coefficients are shown on Fig. 1 (for Q_{CH_4}) and Fig. 2 (for Q_{CO_2}).

Table 3.

Experiment	$K_{X_1CO_2}$	$K_{X_2CO_2}$	Criterion	$K_{X_1CO_2}$ init. cond.	$K_{X_2CO_2}$ init. cond.
1	0.1	10.73	334.1	0.01	0.01
2	0.1	10.73	334.1	0.01	40
3	0.1	10.73	334.1	40	0.01
4	0.1	10.73	334.1	40	40

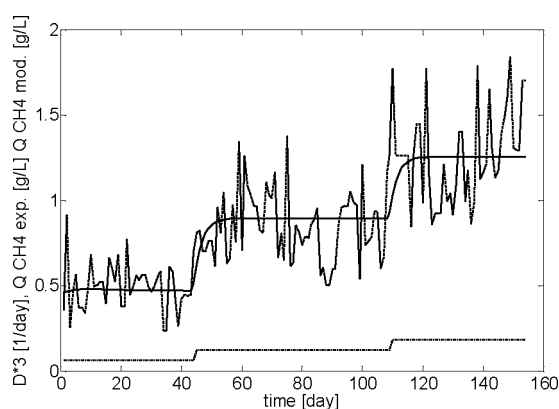


Fig. 1. Experimental (---) and model simulation (—) data for Q_{CH_4} for step change of the input D (—·—) from $D = 0.02$ to $D = 0.04$ and from $D = 0.04$ to $D = 0.06$

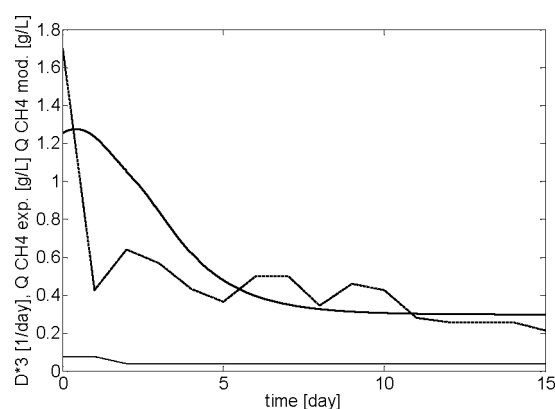


Fig. 3. Experimental (---) and model simulation (—) data for Q_{CH_4} for step change of the input D (—·—) from $D = 0.025$ to $D = 0.0125$

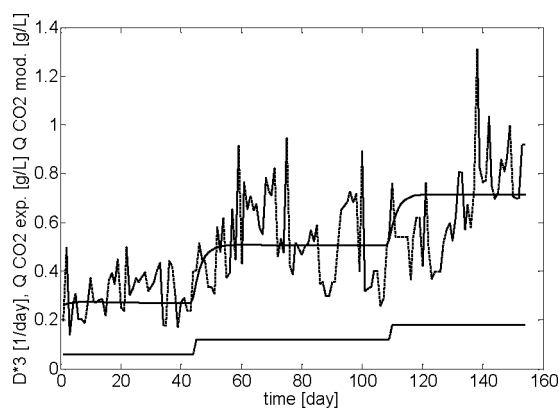


Fig. 2. Experimental (---) and model simulation (—) data for Q_{CO_2} for step change of the input D (—·—) from $D = 0.02$ to $D = 0.04$ and from $D = 0.04$ to $D = 0.06$

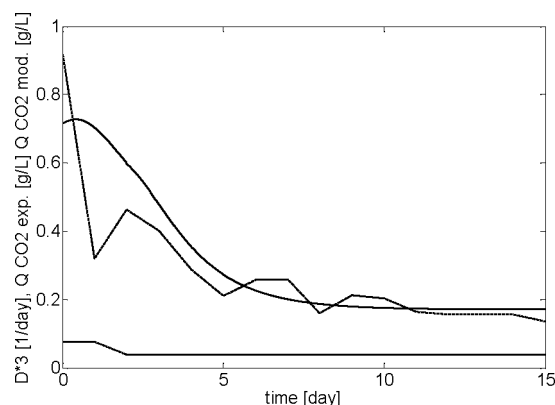


Fig. 4. Experimental (---) and model simulation (—) data for Q_{CO_2} for step change of the input D (—·—) from $D = 0.025$ to $D = 0.0125$

3.3. Model validation

The model validation was made with pilot-scale experimental data for step change of the input D from $D=0.025$ to $D=0.0125$. Some results are shown on Fig. 3 (for Q_{CH_4}) and Fig. 4 (for Q_{CO_2}).

From Fig. 3 to Fig. 6 one may conclude that simulation data for Q_{CH_4} and Q_{CO_2} fit relatively well to the corresponding experimental data.

4. SOFTWARE SENSORS DESIGN

In order to control, or simply monitor, a bioreactor of AD it is necessary to identify and validate the proposed model (1). Identification consists of calculating the constant parameters $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$. This is achieved through a preliminary collection of measurements on the process which have to be large and rich enough to allow the calculation of the previously mentioned parameters. These preliminary measurements are often complex and time consuming ones, implying the use of numerous sophisticated devices.

The next challenge, that is addressed in this section, is to find algorithms, if there are any, which provide online estimations of main dynamic variables of the bioreactor from the previously identified model and easily online measured quantities such as biogas flow rates. Specific growth rates μ_1 and μ_2 are known to be abstract quantities which are introduced; there are no available sensors which are capable to directly measure them. The challenge is actually twofold. First: may quantities such as specific growth rates be estimated in any way? And second: if the answer to the previous question is positive, then devise online estimation schemes for these quantities.

The first question is known in control system literature as observability analysis. Known approaches of observability invoke sophisticated mathematics. This is the case of the approach that is about to be used here to do the observability analysis of the present anaerobic digestion model and for details on the differential algebraic approach of observability and its application to AD [11,12,13]. Using this theory, the characteristic set of the following set of differential polynomials

$$\begin{cases} \dot{S}_0 = -DS_0 - \beta X_1 S_0 + DY_p S_{in} \\ \dot{X}_1 = \mu_1 X_1 - DX_1 \\ Y_1 \dot{S}_1 = -Y_1 DS_1 + \beta Y_1 X_1 S_0 - \mu_1 X_1 \\ \dot{X}_2 = \mu_2 X_2 - DX_2 \\ Y_2 \dot{S}_2 = -Y_2 DS_2 + Y_2 Y_b \mu_1 X_1 - \mu_2 X_2 \\ C \dot{O}_2 = -DCO_2 - Q_{CO_2} + K_{X_1CO_2} \mu_1 X_1 + \\ + K_{X_2CO_2} \mu_2 X_2 \\ Q_{CH_4} = K_{X_2CH_4} \mu_2 X_2 \\ Q_{CO_2} = k_{La} (CO_2 - CO_2^*) \\ CO_2^* = K_H P_C \\ \phi^2 - 4K_H P_T CO_2 = (\phi - 2K_H P_C)^2 \\ k_{La} \phi = k_{La} CO_2 + k_{La} K_H P_T + K_{X_2CH_4} \mu_2 X_2 \end{cases}$$

is calculated with respect to the ranking

$$\left\{ \begin{array}{l} \{\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}\} \\ \{D, S_{in}\} \\ \{Q_{CH_4}, Q_{CO_2}\} \\ \{\mu_1, \mu_2\} \\ \{X_1, X_2\} \\ \{S_0, S_1, S_2, CO_2, \phi, P_C, CO_2^*\} \end{array} \right\}$$

In plain words, the characteristic set algorithm is asked to find, in the following order, relations, if any,

- between the parameters listed in the first line of the above ranking, that is, $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$;
- between the set D, S_{in} and the set of parameters $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$;
- between the set Q_{CH_4}, Q_{CO_2} and the set of all preceding variables, that is, $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}, D, S_{in}$;
- between the set μ_1, μ_2 and the set of all preceding variables, that is, $\beta, P_T,$

$Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4},$
 $D, S_{in}, Q_{CH_4}, Q_{CO_2};$

– between the set X_1, X_2 and the set of all preceeding variables, that is, $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}, D, S_{in}, Q_{CH_4}, Q_{CO_2}, \mu_1, \mu_2;$

– between the set $S_0, S_1, S_2, CO_2, \phi, P_C, CO_2^*$ and the set of all preceeding variables, that is, $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}, D, S_{in}, Q_{CH_4}, Q_{CO_2}, \mu_1, \mu_2, X_1, X_2.$

The result of this calculation is a set of 11 differential polynomials $P_{\mu_1}, P_{\mu_2}, P_{X_1}, P_{X_2}, P_{S_0}, P_{S_1}, P_{S_2}, P_{CO_2}, P_{\phi}, P_{P_C}, P_{CO_2^*}$ introducing [12] the following variables $\mu_1, \mu_2, X_1, X_2, S_0, S_1, S_2, CO_2, \phi, P_C, CO_2^*$ respectively.

Starting with the simplest ones among these differential polynomials, namely

$$P_{\mu_2} = \dot{\mu}_2 Q_{CH_4} + \mu_2^2 Q_{CH_4} - \mu_2 \dot{Q}_{CH_4} - \mu_2 Q_{CH_4} D$$

and

$$P_{X_2} = -\mu_2 X_2 K_{X_2CH_4} D + Q_{CH_4}$$

which reveal the observability [12] of μ_2 and X_2 with respect to $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}, D, S_{in}, Q_{CH_4}, Q_{CO_2}$: the differential algebraic relation between μ_2 and the previous list of variables of least order (and degree) is $P_{\mu_2} = 0$. Therefore μ_2 is not observable [4] with respect to the previous list of variables, but $P_{\mu_2} = 0$ reveals an important fact: μ_2 depends only on D and Q_{CH_4} and not on the model parameters $\beta, P_T, Y_p, Y_b, Y_1, Y_2, k_{La}, K_H, K_{X_1CO_2}, K_{X_2CO_2}, K_{X_2CH_4}$. Moreover, the relation $P_{\mu_2} = 0$ may be transformed into the following one

$$\frac{d}{dt} \left(\frac{Q_{CH_4}}{\mu_2} \right) = -D \left(\frac{Q_{CH_4}}{\mu_2} \right) + Q_{CH_4}$$

which is valid in all time intervals where μ_2 does not identically vanish. Under that condition the quantity $\frac{Q_{CH_4}}{\mu_2}$ is a solution of the differential equation

$$\dot{z}_2 = -Dz_2 + Q_{CH_4}$$

Assuming that D is free of z_2 the previous differential equation is readily a dynamic estimator of μ_2 :

$$\dot{\hat{z}}_2 = -D\hat{z}_2 + \bar{Q}_{CH_4} \quad (3a)$$

$$\hat{\mu}_2 = \frac{\bar{Q}_{CH_4}}{\hat{z}_2} \quad (3b)$$

$$\hat{X}_2 = \frac{\hat{z}_2}{K_{X_2CH_4}} \quad (3c)$$

where the quantity $\bar{Q}_{CH_4}$ is the potentially noisy online measurement of Q_{CH_4} . The estimation error $\tilde{z}_2 = z_2 - \hat{z}_2$ evolves according to the following dynamics

$$\dot{\tilde{z}}_2 = -D\tilde{z}_2 + \tilde{Q}_{CH_4} \text{ with } \tilde{Q}_{CH_4} = Q_{CH_4} - \bar{Q}_{CH_4}$$

In every time interval $[r, s]$, where the quantity D is positive the estimation error exponentially decreases in norm as follows

$$\tilde{z}_2(t) = \tilde{z}_2(r) \exp \left(- \int_r^t D(\sigma) d\sigma \right) + \int_r^t \tilde{Q}_{CH_4}(\sigma) \exp \left(- \int_\sigma^t D(\tau) d\tau \right) d\sigma$$

when t tends to s .

How can the situation of a time interval where μ_2 identically vanishes be detected in practice? And how to set the value of $\hat{\mu}_2$ in that case?

Here is a partial answer to these two questions. According to equation 1g in a time interval where μ_2 identically vanishes Q_{CH_4} identically vanishes, too. Conversely, when Q_{CH_4} identically vanishes in a time interval (or, in practice, given the noise on Q_{CH_4} , when $\bar{Q}_{CH_4}$ is low) then equation 1g shows that the product $\mu_2 X_2$ identically vanishes, and equation 1d shows that X_2 exponentially decays according to $\dot{X}_2 = -DX_2$ unless the input D is maintained to zero in this same time interval in which case X_2 freezes to a constant value. In summary, a time interval with low values of $\bar{Q}_{CH_4}$ is

a presumption of one where μ_2 is unknown but X_2 is certainly either decaying to zero (if, in addition to low values of $\bar{Q}_{CH_4}$, the input D is known to be positive) or freezes to its value at the start of the time interval (if, in addition to low values of $\bar{Q}_{CH_4}$, the input D is known to be zero in the time interval).

Turning to the observability and estimation scheme of μ_1 and X_1 the differential polynomials of the characteristic set which are of interest are P_{μ_1} (which is too large) and P_{X_1} shown below. P_{μ_1} is a quite complex expression of system parameters and variables. But it is found that it takes a simple form which was already encountered in previous works [11,13]. Here is

$$\begin{aligned} P_{X_1} = & -k_{La}K_HK_{X_2CH_4}P_TDQ_{CH_4}Q_{CO_2} - \\ & -k_{La}K_HK_{X_2CH_4}P_TDQ_{CO_2}^2 + \\ & +k_{La}K_{X_1CO_2}K_{X_2CH_4}P_TDQ_{CH_4}^2\mu_1X_1 + \\ & +2k_{La}K_{X_1CO_2}K_{X_2CH_4}Q_{CH_4}Q_{CO_2}\mu_1X_1 + \\ & +k_{La}K_{X_1CO_2}K_{X_2CH_4}Q_{CO_2}^2\mu_1X_1 + \\ & +k_{La}K_HK_{X_2CH_4}P_TQ_{CO_2}\dot{Q}_{CH_4} - \\ & -k_{La}K_HK_{X_2CH_4}P_TQ_{CH_4}\dot{Q}_{CO_2} + \\ & +k_{La}K_{X_2CO_2}Q_{CH_4}^3 - k_{La}K_{X_2CH_4}Q_{CH_4}^2Q_{CO_2} + \\ & +2k_{La}K_{X_2CO_2}Q_{CH_4}^2Q_{CO_2} - K_{X_2CH_4}DQ_{CH_4}^2Q_{CO_2} - \\ & -2k_{La}K_{X_2CH_4}Q_{CH_4}Q_{CO_2}^2 + k_{La}K_{X_2CO_2}Q_{CH_4}Q_{CO_2}^2 - \\ & -2K_{X_2CH_4}DQ_{CH_4}Q_{CO_2}^2 - k_{La}K_{X_2CH_4}Q_{CO_2}^3 - \\ & -K_{X_2CH_4}DQ_{CO_2}^3 - K_{X_2CH_4}Q_{CH_4}^2\dot{Q}_{CO_2} - \\ & -2K_{X_2CH_4}Q_{CH_4}Q_{CO_2}\dot{Q}_{CO_2} - K_{X_2CH_4}Q_{CO_2}^2\dot{Q}_{CO_2} \end{aligned}$$

Lemma1

The differential polynomial equation

$P_{\mu_1} = 0$ takes the form

$$q_1\dot{\mu}_1 - Dq_1\mu_1 + q_1\mu_1^2 - \dot{q}_1\mu_1 = 0 \quad (4)$$

and the differential polynomial equation

$P_{X_1} = 0$ takes the form

$$k_{La}K_{X_1CO_2}K_{X_2CH_4}\mu_1X_1 - q_1 = 0 \quad (5)$$

where

$$\begin{aligned} q_1 = & (k_{La}K_HK_{X_2CH_4}P_TDQ_{CH_4}Q_{CO_2} + \\ & +k_{La}K_HK_{X_2CH_4}P_TDQ_{CO_2}^2 - \\ & -k_{La}K_HK_{X_2CH_4}P_TQ_{CO_2}\dot{Q}_{CH_4} + \\ & +k_{La}K_HK_{X_2CH_4}P_TQ_{CH_4}\dot{Q}_{CO_2} - \\ & -k_{La}K_{X_2CO_2}Q_{CH_4}^3 + k_{La}K_{X_2CH_4}Q_{CH_4}^2Q_{CO_2} - \\ & -2k_{La}K_{X_2CO_2}Q_{CH_4}^2Q_{CO_2} + K_{X_2CH_4}DQ_{CH_4}^2Q_{CO_2} + \\ & +2k_{La}K_{X_2CH_4}Q_{CH_4}Q_{CO_2}^2 - k_{La}K_{X_2CO_2}Q_{CH_4}Q_{CO_2}^2 + \\ & +2K_{X_2CH_4}DQ_{CH_4}Q_{CO_2}^2 + k_{La}K_{X_2CH_4}Q_{CO_2}^3 + \\ & +K_{X_2CH_4}DQ_{CO_2}^3 + K_{X_2CH_4}Q_{CH_4}^2\dot{Q}_{CO_2} + \\ & +2K_{X_2CH_4}Q_{CH_4}Q_{CO_2}\dot{Q}_{CO_2} + K_{X_2CH_4}Q_{CO_2}^2\dot{Q}_{CO_2}) \\ & / (Q_{CH_4} + Q_{CO_2})^2 \end{aligned} \quad (6)$$

The lemma follows from the following two facts:

(i) as a (non differential) polynomial in derivatives of μ_1 , P_{μ_1} is of the form

$$P_{\mu_1} = a_{11}\dot{\mu}_1 + a_{02}\mu_1^2 + a_{01}\mu_1,$$

where a_{11} , a_{02} and a_{01} do not depend on derivatives of μ_1 , and

$$a_{02} = a_{11},$$

(ii) and the coefficient a_{01} turns out to be of the form

$$\frac{a_{01}}{(Q_{CH_4} + Q_{CO_2})^2} = -\dot{q}_1 - Dq_1$$

where q_1 is as in equation 5.

Similarly P_{X_1} is of the form

$$P_{X_1} = b_{01}\mu_1X_1 - b_{00}$$

where

$$b_{01} = k_{La}K_{X_1CO_2}K_{X_2CH_4}(Q_{CH_4} + Q_{CO_2})^2 \text{ and}$$

$$b_{00} = (Q_{CH_4} + Q_{CO_2})^2 q_1.$$

This proves the lemma.

Equations 3 and 4 provide estimation schemes for μ_1 and X_1 similar to equations 2:

$$\begin{cases} \dot{\hat{z}}_1 = -D\hat{z}_1 + \hat{q}_1 & (7a) \\ \hat{\mu}_1 = \frac{\hat{q}_1}{\hat{z}_1} & (7b) \\ \hat{X}_1 = \frac{\hat{z}_1}{k_{La}K_{X_1CO_2}K_{X_2CH_4}} & (7c) \end{cases}$$

where the quantity $\hat{q}_1$ is an estimate of q_1 .

In order to use equation 6b as an estimator for μ_1 it is necessary to properly evaluate the quantity q_1 in equation 5.

If the expression of q_1 taken from equations 5 were to be used as is with experimental data then difficulties would rise from the nonlinear dependency on measurements uncertainties through the time derivatives of Q_{CH_4} and Q_{CO_2} .

Therefore the challenge is to reduce this complex expression of q_1 to a form which is more favorable to online numerical differentiation.

Again, elementary but subtle calculations allow to see that q_1 may be rewritten as

$$\begin{aligned} q_1 = & \left(-k_{La}K_HK_{X_2CH_4}P_TDQ_{CH_4}^2 - k_{La}K_{X_2CO_2}Q_{CH_4}^3 + \right. \\ & + k_{La}K_{X_2CH_4}Q_{CH_4}^2Q_{CO_2} - 2k_{La}K_{X_2CO_2}Q_{CH_4}^2Q_{CO_2} + \\ & + K_{X_2CH_4}DQ_{CH_4}^2Q_{CO_2} + 2k_{La}K_{X_2CH_4}Q_{CH_4}Q_{CO_2}^2 - \\ & - k_{La}K_{X_2CO_2}Q_{CH_4}Q_{CO_2}^2 + 2K_{X_2CH_4}DQ_{CH_4}Q_{CO_2}^2 + \\ & + k_{La}K_{X_2CH_4}Q_{CO_2}^3 + K_{X_2CH_4}DQ_{CO_2}^3 \left. \right) \\ & / (Q_{CH_4} + Q_{CO_2})^2 + k_{La}K_HK_{X_2CH_4}P_TD + \\ & + k_{La}K_HK_{X_2CH_4}P_T \left(\frac{1}{1 + \frac{Q_{CH_4}}{Q_{CO_2}}} \right) + K_{X_2CH_4}\dot{Q}_{CO_2} \end{aligned}$$

5. SIMULATION STUDIES

Simulation studies using *Simulink toolbox* of *Matlab* were performed with the previous estimation schemes for step changes of the dilution rate shown on Fig. 5. The performance of the estimation schemes is compared to the mass balance model (1).

The simulation results are presented in the Fig. 6 to 9 for step-wise changes shown in Fig. 5. Fig. 10 presents the flow rates of CO_2 and CH_4 .

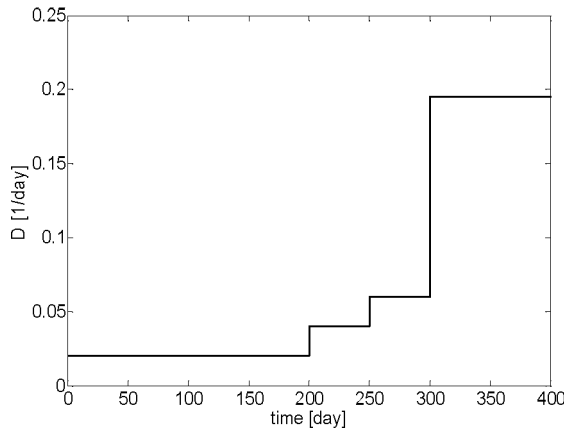


Fig. 5. Dilution rate

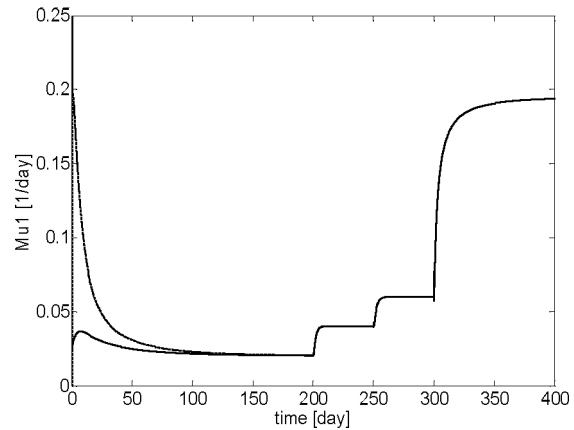


Fig. 6. Specific growth rate of acidogenic bacteria:
 $\mu_1(-)$, $\hat{\mu}_1(- -)$

The estimation of the state variables is easy to implement. It provides good convergence behavior for μ_2 and X_2 (about 25 days) and it is quite slow for μ_1 and X_1 (about 50 days and more). This could be corrected slightly with the appropriate choice of the initial conditions of the integrators. For

continuous processes the slow convergence is not a problem. This technique could provide reliable and cheap sensors for online monitoring and control of the AD process. As a perspective, validation of the estimation strategy on experimental data could be performed.

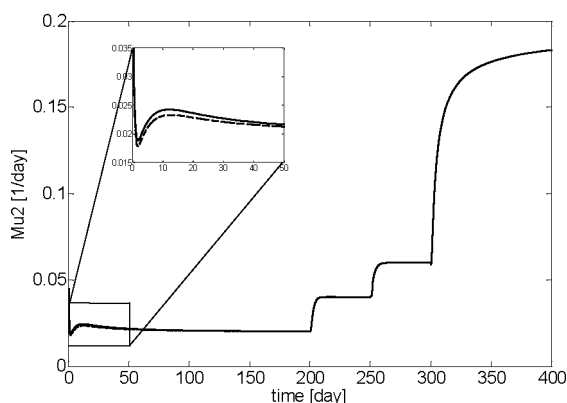


Fig. 7. Specific growth rate of methanogenic bacteria: $\mu_2(-)$, $\hat{\mu}_2(- -)$

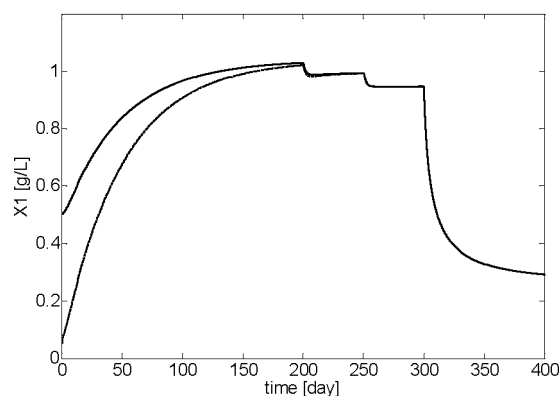


Fig. 9. Methanogenic bacteria concentration: $X_2(-)$, $\hat{X}_2(- -)$

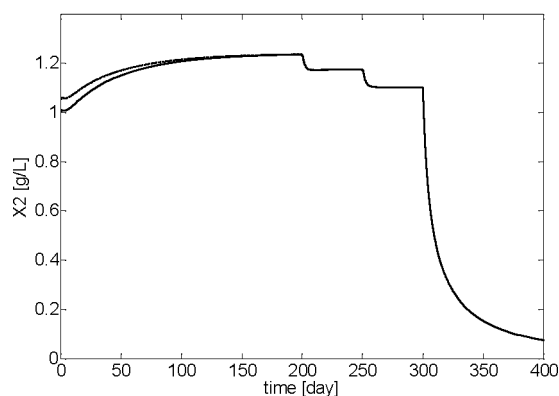


Fig. 8. Acidogenic bacteria concentration: $X_1(-)$, $\hat{X}_1(- -)$

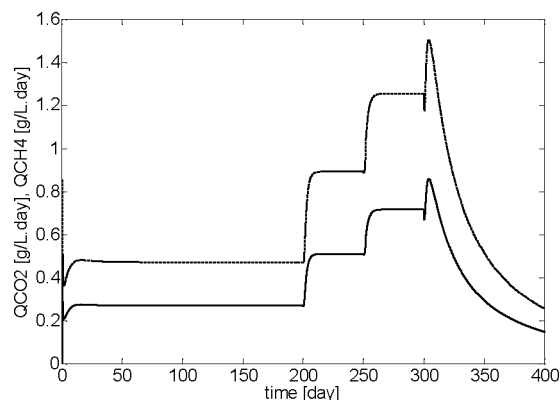


Fig. 10. $CO_2(-)$ and $CH_4(- -)$ flow rates

6. CONCLUSION

In this paper a modification, concerning the gas-phase modeling, of the simple mathematical model of AD from [9] was developed and verified experimentally. The following points are important, because they guarantee that our model can be useful to monitor and control the AD process:

1. It is based on mass-balance considerations.
2. Two-step identification procedure to estimate 3 model parameters was used on the base of the independence of experimental data for dynamics of the specific methane flow-rate and for the specific carbon dioxide flow-rate.
3. Unique solutions were obtained for all coefficients.
4. The validation of the model was performed using pilot scale experimental data.

On the base of the modified simple mathematical model of the AD software sensors using the differential algebraic approach were designed and studied by simulations.

In the present paper it was proposed to eliminate this additional modeling effort on specific growth rates by simply providing an estimation scheme for these specific growth rates based on easily available measurements such as gas flow rates, percentages of methane and carbon dioxide in the biogas together with measurements of dissolved carbon dioxide. The interest of this contribution is not only to save the time and effort to identify empirical models, but our result allows to easily modify the waste composition without having to re do such empirical model identification.

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МОДЕЛИРАНЕ И РАЗРАБОТВАНЕ НА СОФТУЕРНИ СЕНЗОРИ ЗА ПРОЦЕС НА АНАЕРОБНА БИОДЕГРАДАЦИЯ

Е. Чорукова, С. Диоп, И. Симеонов, С. Тебани

Резюме. Анаеробното разграждане е ефективен биотехнологичен процес за обработка на различни селскостопански, битови и промишлени отпадъци. Използването на математически модели е мощен инструмент за изследване и оптимизиране на процесите на анаеробна биодегradация (АБД), както и за разработване на софтуерни сензори. В тази статия е разработена и проверена експериментално нова версия, отнасяща се до моделиране на газова фаза на упростен математически модел на АБД. Параметричната идентификация се основава на 150-дневен набор от динамични експерименти в лабораторен биореактор. Представена е двустъпална процедура за идентификация на 3 параметъра на модела. Данните от 15-дневен експеримент на пилотен биореактор са използвани за валидиране на модела.

На основата на модифицирания упростен математически модел на а АБД и използвайки диференциално-алгебричен подход, са разработени и симулационно изследвани софтуерни сензори.

Ключови думи: анаеробна биодегradация, математическо моделиране, оценяване на специфични скорости на растеж, теория за наблюдение и управление на системи.

Елена Чорукова

Институт по микробиология "Стефан Ангелов", БАН
Ул. "Акад. Г. Бончев" бл. 26, София 1113
E-mail: elena@microbio.bas.bg

Sette Diop

Laboratoire des Signaux & Systèmes,
CNRS-CentraleSupélec, 91192 Gif sur Yvette cedex France
E-mail: diop@l2s.centralesupelec.fr

Иван Симеонов

Институт по микробиология "Стефан Ангелов", БАН
Ул. "Акад. Г. Бончев" бл. 26, София 1113
E-mail: issim@abv.bg

Sihem Tebbani

Laboratoire des Signaux & Systemes, CentraleSupélec, France
CNRS-CentraleSupélec, 91192 Gif sur Yvette cedex France
E-mail: sihem.tebbani@centralesupelec.fr

