*BIO*AUTOMATION, 2009, 12, 88-105

Parameter and State Estimation of an Anaerobic Digestion of Organic Wastes Model with Addition of Stimulating Substances

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Received: January 20, 2009 **Accepted: February 27, 2009**

Published: March 16, 2009

Abstract: *New control inputs are introduced in the 5th order mass-balance non-linear model of the anaerobic digestion, which reflects the addition of stimulating substances (acetate and glucose). Laboratory experiments have been done with step-wise and pulse changes of these new inputs. On the basis of the step responses of the measured variables (biogas flow rate and acetate concentration in the bioreactor) and iterative methodology, involving non-linear optimisation and simulations, the model coefficients have been estimated. The model validity has been proved by another set of experiments. The observation part is built on a two-step structure. One estimator and two observers are designed on the basis of this process model. Their stability has been proved and their performances have been investigated with experimental data and simulations.*

Keywords: *Anaerobic digestion, Acetate and glucose supply, Non-linear model, Parameter and state estimation.*

Introduction

In the biological anaerobic wastewater treatment processes (anaerobic digestion) the organic matter is mineralised by micro-organisms into biogas (methane and carbon dioxide) in absence of oxygen. The biogas is an additional energy source and the methane is a greenhouse gas. In general these processes are carried out in continuous stirred tank bioreactors (CSTR). Anaerobic digestion (AD) has been widely used in life process and has been confirmed as a promising method for solving some energy and ecological problems in agriculture and agro-industry. Unfortunately this process sometimes is a very unstable one and need more investigations. Livestock manure is a complex substrate and its anaerobic degradation consists of a complex series of reactions catalysed by a consortium of different bacteria [1, 4, 10]. Volatile fatty acids (VFA) are the most important intermediates for methanogenesis. Consequently, the process can be regarded as a process where accumulation of acetate and higher VFA is the most noticeable result of process stress [1, 10]. Codigestion of several wastes (manure, sewage sludge and wastes from food processing industry) is

another environmentally attractive method for 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 [2]. Recent investigations show that addition of stimulating substances (acetate or glucose) in appropriate concentrations stabilize the process and increase the biogas flow rate [13, 21].

Mathematical modelling represents a very attractive tool for studying this process [2-5, 7], however a lot of models are not appropriate for control purposes due to their complexity. The choice of relatively simple models of this process, theirs parameters estimation and design of software sensors for the immeasurable variables on the basis of an appropriate model is a very important step for realisation of sophisticated control algorithms [6, 8, 11, 12, 19].

The aim of this paper is twofold:

- to estimate the coefficients of a 5^{th} order non-linear model of the anaerobic digestion with addition of acetate and glucose as stimulating substances, which may be viewed as new control inputs (influent acetate or glucose concentrations or flow rates);
- on the basis of this model to design stable estimators of the growth rates and observers of the concentrations of the two main groups of micro-organisms (acidogenic and methanogenic), appropriate for future control purposes.

Process model and parameter estimation

Experimental design and experimental studies

The laboratory experimental set-up includes an automated bioreactor of a 3 l glass vessel developed and adapted to fulfil the requirements for anaerobic digestion. It is mechanically stirred by electrical drive and maintained at a constant temperature $(34\pm0.5)^0$C. The monitoring of the methane reactor is carried out by data acquisition computer system of on-line sensors, which provide the following measurements: pH, temperature (t), speed of agitation and biogas flow rate (Q).

Laboratory experiments are carried out in the bioreactor with highly concentrated organic pollutants (cattle dung and mixtures of cattle dung and sewage sludge) including addition of acetate and glucose in appropriate concentrations. Sampling frequency – as in the real life AD processes all manipulations have been done once a day with constant sampling and injection time. Experiments resemble the situation under which the model is to be used. However some more specific experiments with excitation signals for model calibration and validation have been performed. Excitation signals (perturbing the process in such a way that highly qualitative information has been gathered) as a step-wise functions and additional pulses (with increasing amplitude from 0.5 $g\cdot l^{-1}$ to 3.5 $g\cdot l^{-1}$ by steps of 0.25 $g\cdot l^{-1}$) have been adopted. The responses of Q and S_2 are obtained for step-wise and pulse changes of the acetate and glucose addition. S_2 is determined by gas chromatography. The length of the experiments has been determined by the time necessary to reach the steady-state after each step change of the input action. After performing start-up of the process, appropriate steady-state in continuous mode of operation has been reached following previous knowledge [15, 16]. It has been experimentally proved that step-wise and pulse addition of acetate and glucose must be bounded in amplitude.

However it is well known that the anaerobic digestion has the following characteristics [1, 2, 4]:

- the pH in the bioreactor is strongly influenced by the volatile fatty acids (VFA) produced (in our case mainly acetate) – the accumulation of VFA depresses pH;
- self-stabilization of the process will occur and total failure will be prevented, unless the disturbance is of a magnitude exceeding the buffer capacity of the medium, i.e. pH breakdown before stabilization occurs.

That means that acetate addition into the anaerobic bioreactor will increase the biogas production, however pH breakdown is possible. A lot of experiments in laboratory and pilot plants [1, 13] show that during digestion of cattle manure violent pH changes or sudden process failure does not occur, due to the high buffering capacity of manure [1]. That is why after a lot of laboratory experiments [13] the following proposal to overcome this problem has been elaborated: after obtaining the admissible range of the concentrations for acetate or glucose added into the anaerobic bioreactor operating with wastes different by its nature, pH regulation (correction till pH = 8.5) of the inlet mixture must be done.

The acetate and glucose feed rates (concentration multiplied by dilution rate) may be introduced as additional control inputs. However from experimental investigation the following conclusion has been drown – both the quantity of the acetate (glucose) added into the bioreactor and its rate of change must be bounded due to possible inhibitory effects.

Mathematical modelling of the process

On the basis of the above-presented experimental investigations and following the so-called three-stage biochemical scheme of the AD [4], the following 5th order non-linear model with three control inputs is proposed [21]:

$$\frac{dS_0}{dt} = -\beta X_1 S_0 + D_1 Y_p S_{0i} - DS_0 \tag{1}$$

$$\frac{dX_1}{dt} = \left(\mu_1 - D\right) X_1 \tag{2}$$

$$\frac{dS_1}{dt} = -\mu_1 \frac{X_1}{Y_1} + \beta X_1 S_0 + C_k D_2 S_{10}^{"} - DS_1 \tag{3}$$

$$\frac{dX_2}{dt} = \left(\mu_2 - D\right) X_2 \tag{4}$$

$$\frac{dS_2}{dt} = -\mu_2 \frac{X_2}{Y_2} + Y_b \mu_1 X_1 + D_3 S_{20}^{"} - DS_2 \tag{5}$$

$$Q = k_4 \mu_2 X_2 \tag{6}$$

For the non-linear functions μ_1 and μ_2 the following structures are adopted:

$$\mu_1 = \frac{\mu_{1\max} S_1}{k_{S1} + S_1 + S_1^2 / k_{i1}} \; ; \; \mu_2 = \frac{\mu_{2\max} S_2}{k_{S2} + S_2 + S_2^2 / k_{i2}} \tag{7}$$

In this mass balance model Eq. (1) describes the hydrolysis in a very simple way [4], where the first term reflects the hydrolysis of the diluted organics by acidogenic bacteria, the second term – the influent flow rate of liquid with concentration of the diluted organics S_{0i}, [g·l^{-1}]

and the third one – the effluent flow rate of liquid. Eq. (2) describes the growth and changes of the acidogenic bacteria (with concentration X_1, [g·l^{-1}]), consuming the appropriate substrate (with concentration S_1, [g·l^{-1}]). The mass balance for this substrate is described by (3), where the first term reflects the consumption by the acidogenic bacteria, the second term – the substrate S_1, [g·l^{-1}] formed as a result of the hydrolysis, the third one – the direct addition of glucose (with concentration $S_{10}^{"}$, [g·l^{-1}]) and the last one – the substrate S_1, [g·l^{-1}] in the effluent flow rate of liquid. Eq. (4) describes the growth and changes of the methane producing (methanogenic) bacteria (with concentration X_2, [g·l^{-1}]), consuming acetate (with concentration S_2, [g·l^{-1}]). The mass balance equation for acetate (5) has four terms in his right side. The first one reflects the consumption of acetate by the methanogenic bacteria, the second – the acetate formed as a result of the activity of acidogenic bacteria, the third one – the direct addition of acetate (with concentration $S_{20}^{"}$, [g·l^{-1}]) and last one – the acetate in the effluent liquid. The algebraic Eq. (6) describes the formation of biogas (with flow rate Q in [l gas/l medium per day]). The relations (7) present the specific growth rate of the acidogenic bacteria μ_1, [day^{-1}] (known as Haldane type and reflecting a possible inhibition by high concentration of glucose) and the specific growth rate of the methanogenic bacteria μ_2, [day^{-1}] (reflecting a possible inhibition by high concentration of acetate). β, Y_p, Y_1, Y_2, Y_b, k_4, μ_{max1}, μ_{max2}, k_{s1}, k_{s2}, k_{i1} and k_{i2} are coefficients, D_1, [day^{-1}] is the dilution rate for the inlet soluble organics (with concentration S_{0i}), D_2, [day^{-1}] is the dilution rate for glucose (with concentration $S_{10}^{"}$, [g·l^{-1}]), D_3, [day^{-1}] is the dilution rate for the acetate (with concentration $S_{20}^{"}$, [g·l^{-1}]) added into the bioreactor and $D = D_1 + D_2 + D_3$, [day^{-1}] is the total dilution rate.

In this model S_{0i} is generally an immeasurable (on line) perturbation, while Q and S_2 are measurable outputs, D_1, D_2 and D_3 are control inputs, $S_{10}^{"}$ and $S_{20}^{"}$ are known constants or control inputs. In all cases the washout of micro-organisms (for $D \geq D^{sup}$) and acetate or glucose inhibitions are undesirable, that is why changes of the control input D and the perturbation S_{0i} are possible only in some admissible ranges (for fixed values of $S_{10}^{"}$ and $S_{20}^{"}$):

$$0 \leq D \leq D^{sup}$$

$$S_{0i}^{inf} \leq S_{0i} \leq S_{0i}^{sup}$$

$$D_2 \; S_{10}^{"} < M_1 \, , \; \left| \frac{dD_2}{dt} \right| \leq M_2$$

$$D_3 \; S_{20}^{"} < M_3 \, , \; \left| \frac{dD_3}{dt} \right| \leq M_4$$

where M_i (i = 1, 2, 3, 4) are constants.

In our case (digestion of cattle manure and mixtures of cattle manure and sewage sludge) the following values of these boundary constants are experimentally obtained: D^{sup} = 0.1 day^{-1}, M_1 = 1.3 g·l^{-1}·day^{-1}, M_2 = 0.25 g·l^{-1}·day^{-1}, M_3 = 1.5 g·l^{-1}·day^{-1}, M_4 = 0.3 g·l^{-1}·day^{-1} for variation of S_{0i} in the range 30 - 70 g·l^{-1}.

Parameter estimation

Dynamic modelling makes sense only if the coefficients of the models have well-specified numerical values. Since the coefficients in the model (1) to (7) are generally not known a priori (only some ranges for their values are known [20]), they need to be estimated from experimental data. Unfortunately the identifiability of these coefficients is far from being guarantied, because very different sets of coefficients can provide quite similar simulation results which fit the data equally well [12, 14-17].

For the above presented model different sets of coefficients are obtained for particular kinds of digested organic matter [8, 15, 20]. In the case of new manipulated inputs it has been necessary to precise some coefficients in the model. In this paper without searching the identifiability (structural or/and practical) of the model parameters (a very difficult problem [20]) a multi-step iterative approach and expert knowledge have been applied to solve this problem.

The estimation of the coefficients of the above presented model is a very difficult problem, because of the rather restricted information - usually only the concentration of acetate (S_2) and the biogas production rate (Q) can be measured (for known influent organic concentration (S_{0i}) and some data for the glucose concentration in the bioreactor). In some cases a careful planning and performing of batch and fed-batch experiments allow accurate estimation of μ_m and k_s, in Monod-type kinetic expressions [14]. However this result is obtained with very restrictive assumption (constant biomass concentration) and only for Monod-type kinetics. In this paper a simple iterative methodology for model parameter estimation is proposed on the basis of sensitivity analysis and non-linear optimisation methods. It consists in the following steps:

1. The responses of all measurable values are taken down under appropriate excitation signals (step-wise and impulse changes in our case) of the appropriate input (in the admissible ranges) during the experimental studies.
2. Determination of (some) unknown initial values of the state variables using optimisation method.
3. Separation of the unknown coefficients into two (or more) groups using sensitivity analysis.
4. Estimation of the first (more sensitive) group of coefficients with arbitrary known other coefficients using optimisation method and appropriate criterion.
5. Estimation of the second group of coefficients with the above determined values of the first group using optimisation method and appropriate criterion.
6. Model verification with the above obtained coefficients and another set of experimental data.
7. Restart with point 2 if some coefficients estimates are not satisfying.

The responses of Q and S_2 have been taken down for step changes of $S_{10}^{"}$ (or $S_{20}^{"}$), when D_1. D_2 (or D_3) and S_{0i} have been kept constants. A sensitivity analysis with respect to ten coefficients have been made only on the basis of simulation studies and they were divided into the following two groups: Y_i (yield coefficients) in the first group, μ_{max1}, μ_{max2}, k_{s1}, k_{i1}, k_{s2} and k_{i2} in the second group. Applying the above presented methodology the parameters estimation starts with the first (more sensitive) group of coefficients with known initial values of all coefficients obtained from other experiments (without acetate addition [16]). Estimation of the second group of coefficients with the above-determined values of the first group is the

following step, etc. These manipulations have been performed with experimental data obtained when acetate or glucose have been injected (not simultaneously) to independently characterize the two main groups of anaerobic microorganisms.

A schematic diagram of the used non-linear identification method is shown on Fig. 1. In this case the following criterion was applied:

$$J_6 = \Sigma C_1[S_{2\exp}(i) - S_{2m}(i)]^2 + C_2[Q_{\exp}(i) - Q_m(i)]^2 \Rightarrow min \quad (8)$$

C_i – weight coefficients (generally $C_i = 1$).

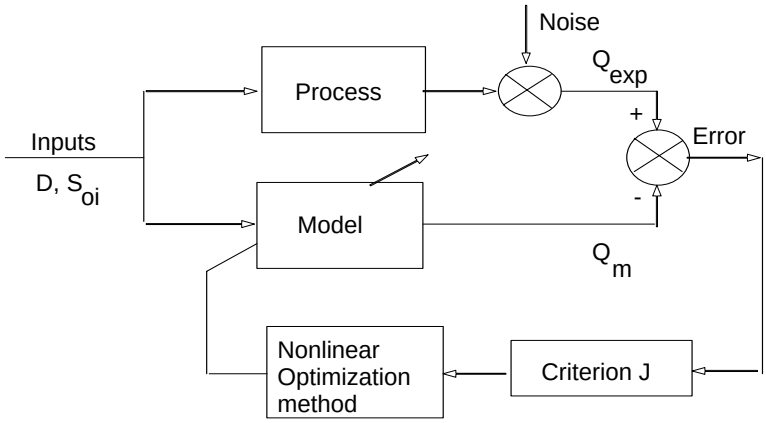


Fig. 1 Non-linear identification method

All optimisation methods of the Optimisation Toolbox (MATLAB) may be used with generated data from a known model (with and without measurement noise on Q and S_2) but only two of them (Simplex Search and Marquardt-Levenberg) have presented good performances for the non-linear identification task. In our case the best results of the model parameters estimation were obtained using Simplex Search method with smoothed data and $C_1 = 1$, $C_2 = 1$. Since prior knowledge about initial parameter values is essential in solving non-linear estimation problems (to avoid biased estimates to a large extent), the start has been performed with initial values know from our previous work [16]. The final results are summarised in Table 1.

Table 1

β	Y_p	μ_{max1}	μ_{max2}	k_{s1}	k_{s2}	Y_1	Y_2	Y_b	k_4	k_{i2}	k_{i1}	C_k
3	0.144	0.4	0.25	1.9	0.37	0.15	0.24	5	3.0	1.5	0.935	0.4

Model validation

Some experimental and simulation results are compared on Fig. 2 and Fig. 3. On Fig. 2 evolutions of X_1, X_2, S_1, S_2, S_{2exp}, Q and Q_{exp} for 13 days are presented in the case of one step addition of acetate (S''_{20} from 0 to 25 g·l^{-1}) and S_{0i} = 68 g·l^{-1}, D_1 = 0.0375 day^{-1} and D_2 = 0.0125 day^{-1}. Evolutions of X_1, X_2, S_1, S_2, Q and Q_{exp} for 35 days are presented on Fig. 3 in the case of three step additions of acetate (S''_0 = 25 g·l^{-1} from t = 0 to 6; S''_{20} = 50 g·l^{-1} from t = 7 to 16; S''_{20} = 75 g·l^{-1} from t = 17 to 35) for D_1 = 0.0375 day^{-1}, D_2 = 0.0125 day^{-1} and

S_{0i} = 75 g·l^{-1}. Experimental data for D_2 = 0.0125 day^{-1} with the first step change of $S_{20}^{"}$ (from 0 to 25 g·l^{-1}) and S_{0i} = 68 g·l^{-1} have served for parameter estimation. The model validation for obtained parameters has been performed with different step and impulse changes of the acetate and glucose added into the anaerobic bioreactor and different values of S_{0i}. This is illustrated on Fig. 3 – experimental data for D_2 = 0.0125 day^{-1} with the 2nd and 3rd step changes of $S_{20}^{"}$ (from 25 to 50 g·l^{-1} and from 50 to 75 g·l^{-1}) with S_{0i} = 75 g·l^{-1} have been kept for model validation. Our conclusion is that the behaviour of the model with the new control inputs is satisfying comparing to the process one.

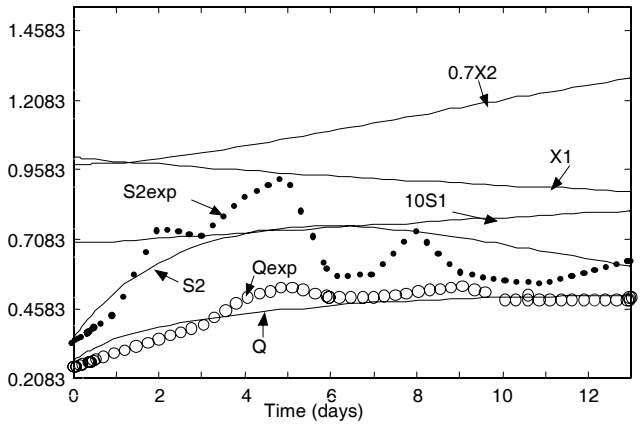


Fig. 2 Evolution of X_1, X_2, S_1, S_2, S_{2exp}, Q and Q_{exp}
in the case of one step addition of acetate and S_{0i} = 68 g·l^{-1}

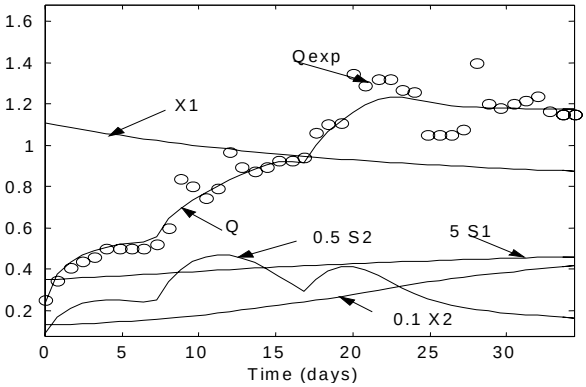


Fig. 3 Evolution of X_1, X_2, S_1, S_2, Q and Q_{exp}
in the case of three step additions of acetate and S_{0i} = 7.5 g·l^{-1}

State estimation

Problem statement

For the model (1) – (7) it is assumed that:

A1. The growth rates $R_1 = \mu_1 X_1$ and $R_2 = \mu_2 X_2$ associated to acidogenic and methanogenic bacteria respectively, are unknown time-varying parameters, which are nonnegative and bounded, with bounded time derivative.

A2. The concentrations of X_1, X_2, S_1, cannot be measured on-line, while methane production rate Q and acetate concentration S_2 are measured on-line.

For the model (1) – (7) under the assumptions A1-A2, the following problem is considered: design an estimator of the growth rate R_1 and observers of the concentrations X_1 and X_2, using on-line measurements of Q and S_2.

Since for the considered process only the concentrations of substrate for methanogenic bacteria, S_2 (acetate) and the biogas flow rate, Q, are on-line measured, it is evident that the process is not observable from the available measurements and therefore an observer estimating simultaneously the growth rate of acidogenic bacteria concentration, R_1, acidogenic and methanogenic bacteria concentrations, X_1, and X_2, and the corresponding specific growth rates, can not be designed. For this reason, in this paper, a two step approach for estimation of above mentioned parameters and variables is proposed.

In first step, an observer based estimator of the growth rate of acidogenic bacteria concentration, R_1, is derived using the available on-line measurements. Also, at this step, an idea, proposed in [9] is applied for the design of an observer of acidogenic bacteria concentration in the considered complex process. This idea is related to the cases when the estimated variable is not observable from measured one and consists in the introduction of auxiliary time-varying parameter, with the help of which the observability problem can be resolved.

The second step of the estimation approach includes the design of an observer of methanogenic bacteria concentration using the same idea, however with the available measurements of S_2 and Q, and additionally (in comparison to the observer of acidogenic bacteria concentration from the first step) the estimates of growth rate of acidogenic bacteria concentration, obtained on previous step, which are considered as on-line measurements.

The obtained estimates of X_1, X_2, R_1 and the indirect R_2 measurement, give the possibility to be obtained on-line estimates of the specific growth rates, μ_1 and μ_2.

Estimator and observer design for the acidogenic stage

Estimator of the growth rate R_1

We assumed that:

A3. Noisy measurements Q_m and S_{2m} are available on-line:

$$Q_m = Q + \varepsilon_1;\ S_{2m} = S_2 + \varepsilon_2$$

where ε_1 and ε_2 are measurements noises.

The following observer-based estimator of R_1 is proposed using the dynamical Eq. (5) of S_2 concentration:

$$\frac{d\hat{S}_2}{dt} = -DS_{2m} + k_3\hat{R}_1 - k_2R_{2m} + C_{1R1}(S_{2m} - \hat{S}_2)$$
$$\frac{d\hat{R}_1}{dt} = C_{2R1}(S_{2m} - \hat{S}_2) \quad (9)$$

where $R_{2m} = Q_m/k_4 = R_2 + \varepsilon_1/k_4$ are measured values of R_2, ε_1/k_4 represents a measurement noise of R_2 and C_{1R1}, C_{2R1} are estimator parameters.

The X_1 estimates are obtained by:

$$\dot{\hat{X}}_{1m} = \hat{R}_1 - D\hat{X}_{1m} \quad (10)$$

where $\hat{R}_1$ is the estimate of R_1 obtained by estimator (9), while the μ_1 estimate can be derived on the basis of the relationship:

$$\hat{\mu}_{1m} = \hat{R}_1 / \hat{X}_{1m} \quad (11)$$

Stability analysis

Consider the error system associated to the observer

$$\frac{dx}{dt} = Ax + u \quad (12)$$

$$x = \begin{vmatrix} \tilde{S}_2 \\ \tilde{R}_1 \end{vmatrix} = \begin{vmatrix} S_2 - \hat{S}_2 \\ R_1 - \hat{R}_1 \end{vmatrix}; \; A = \begin{vmatrix} -C_{1R1} & k_3 \\ -C_{2R1} & 0 \end{vmatrix}; \; u = \begin{vmatrix} D\varepsilon_2 + k_2\dfrac{\varepsilon_1}{k_4} - C_{1R1}\varepsilon_2 \\ -C_{1R1}\varepsilon_2 + \dfrac{dR_1}{dt} \end{vmatrix}$$

where x is the estimation error vector, u is the input vector of the error system and A is the matrix of the error system. The values of C_{1R1}, C_{2R1} have to be chosen such that matrix A remains stable, i.e., $C_{1R1} > 0$ and $C_{2R1} > 0$.

Observer of X_1

The X_1 estimates, obtained by (10) have the disadvantage that the speed of convergence is limited by experimental condition through the dilution rate D. To improve the convergence rate and consequently the estimation accuracy, a "software sensor" of X_1 is derived. The observer design is based on the dynamical equation of measured variable S_2, obtained by (5). Since in this equation μ_1 is considered as unknown time-varying parameter, the variable X_1 is not observable. For this reason, the idea, proposed in [9] is applied for the observer design. This idea consists in the introduction of auxiliary time-varying parameter with aim to be overcome the observability problem.

The dynamics of S_2 (5) is considered and the following auxiliary parameter is defined:

$$\varphi_1 = R_1 + \lambda_1 X_1, \quad (13)$$

where λ_1 is a bounded positive real number. Substituting R_1 from (13) in the dynamical equation of S_2 (5), the following observer of X_1 is derived:

$$\begin{aligned}
\frac{d\hat{S}_2}{dt} &= -DS_{2m} + k_3\hat{\varphi}_1 - k_3\lambda_1\hat{X}_1 - k_2R_{2m} + D_2S_0'' + C_{1X1}(S_{2m} - \hat{S}_2) \\
\frac{d\hat{X}_1}{dt} &= \hat{\varphi}_1 - (D+\lambda_1)\hat{X}_1 + C_{2X1}(S_{2m} - \hat{S}_2) \\
\frac{d\hat{\varphi}_1}{dt} &= C_{3X1}(S_{2m} - \hat{S}_2)
\end{aligned} \tag{14}$$

where C_{1X1}, C_{2X1}, C_{3X1} are observer parameters.

The speed of convergence of the X_1 estimates, to the true ones can be improved (in comparison to the Eq. (10)) by an appropriate choice of the observer parameters C_{1X1}, C_{2X1} and C_{3X1}.

Therefore, more accurate estimates of the specific growth rate μ_1 (in comparison with those derived from (11)) can be obtained using the kinetic model:

$$\hat{\mu}_1 = \hat{R}_1 / \hat{X}_1, \tag{15}$$

where $\hat{R}_1$ are the estimates of R_1 obtained from (9) and $\hat{X}_1$ are the estimates of X_1, obtained by observer (14).

Stability analysis

Consider the dynamics of the estimation error (12). In the considered case, the values of the matrix and vectors are:

$$x = \begin{vmatrix} \tilde{S}_2 \\ \tilde{X}_1 \\ \tilde{\varphi}_1 \end{vmatrix}; \; A = \begin{vmatrix} -C_{1X1} & -\lambda_1 k_3 & k_3 \\ -C_{2X1} & -D-\lambda_1 & 1 \\ -C_{3X1} & 0 & 0 \end{vmatrix}; \; u = \begin{vmatrix} -C_{1X1}\,\varepsilon_2 - D\varepsilon_2 - k_2\varepsilon_3 \\ -C_{2X1}\,\varepsilon_2 \\ -C_{3X1}\,\varepsilon_2 + \dot{\varphi}_1 \end{vmatrix} \tag{16}$$

where $\varepsilon_3 = R_{2m} - R_2$ is estimation error of R_2.

Case 1: D constant

In this case on the basis of the Hurvitz stability criterion [18] the following sufficient conditions for stability are obtained (for $\lambda_1 > 0$):

$$C_{1X1} > 0;\; C_2X_1 < 0;\; C_{3X1} > 0; \tag{17}$$

Case 2: D variable

The following sufficient conditions were obtained by the second Liapunov method as:

$$\begin{aligned}
&C_{1X1} > (-C_{3X1}a_4 - C_{2X1}a_5)/a_1; \\
&C_{2X1} = \{-a_1k_3\lambda_1 - a_5(D + \lambda_1 + C_{1X1})\}/a_2;
\end{aligned} \tag{18}$$

$C_{3X1} = (-C_{1X1}a_4 + a_5 + k_3a_1)/a_3$

where: a_1, a_2, a_3 are positive constants, a_4 and a_5 are negative constants, satisfying the relations:

$$a_1a_2 > a_5^2;\ a_1a_2a_3 - a_2a_4^2 - a_3a_5^2 > 0;\ a_2 = a_4k_3\lambda_1 - k_3a_5;\ -a_2(D + \lambda_1)/k_3\lambda_1 < a_5 \quad (19)$$

Estimator and observer design for the methanogenic stage

A possible solution to the estimation problem of X_2 is connected to the integration of the following equation:

$$\dot{\hat{X}}_{2m} = R_{2m} - D\hat{X}_{2m}, \quad (20)$$

where R_{2m} are the measured values of R_2, obtained using the relationship:

$$R_{2m} = Q_m/k_4 \quad (21)$$

The estimation of the specific growth rate μ_2 can be realised from the kinetic model:

$$\hat{\mu}_{2m} = R_{2m} / \hat{X}_{2m} \quad (22)$$

Similarly to (10), the convergence rate of X_2 estimates to its true values in (20) is completely determined by the experimental conditions. A new observer of X_2 is proposed to improve the convergence speed of the estimate to its true values as well as to reduce the influence of the measurement noises on the accuracy of the estimation. The observer design is based on the dynamical equation of S_2. Since μ_2 is considered as unknown time-varying parameter, the variable X_2 is not observable from S_2 measurements. Analogously to the X_1 observer, the idea, proposed in [9] is applied to resolve this problem introducing the following auxiliary time-varying parameter:

$$\varphi_2 = R_2 + \lambda_2 X_2, \quad (23)$$

where λ_2 is a bounded real number.

By combining (23) and (5), it is possible to propose the following adaptive observer of X_2:

$$\begin{aligned}
\frac{d\hat{S}_2}{dt} &= -DS_{2m} - k_2\hat{\varphi}_2 + k_2\lambda_2\hat{X}_2 + k_3R_{1m} + D_2S_0'' + C_{1X2}(S_{2m} - \hat{S}_2) \\
\frac{d\hat{X}_2}{dt} &= \hat{\varphi}_2 - (D+\lambda_2)\hat{X}_2 + C_{2X2}(S_{2m} - \hat{S}_2) \\
\frac{d\hat{\varphi}_2}{dt} &= C_{3X2}(S_{2m} - \hat{S}_2)
\end{aligned} \quad (24)$$

where C_{1X2}, C_{2X2} C_{3X2} are observer parameters and R_{1m} is the estimate of R_1 obtained by estimator (9).

Like μ_1, more accurate estimates of the specific growth rate μ_2 (in comparison with the one derived from (22)) can be obtained using the kinetic model:

$$\hat{\mu}_2 = R_{2m} / \hat{X}_2 \tag{25}$$

where $\hat{X}_2$ are the estimates of X_2, obtained by (24).

Stability analysis

Consider the dynamics of the estimation error (12). In the considered case, the values of the matrix and vectors are:

$$x = \begin{vmatrix} \tilde{S}_2 \\ \tilde{X}_2 \\ \tilde{\varphi}_2 \end{vmatrix}; \; A = \begin{vmatrix} -C_{1X2} & -\lambda_2 k_2 & -k_2 \\ -C_{2X2} & -D-\lambda_2 & 1 \\ -C_{3X2} & 0 & 0 \end{vmatrix}; \; u = \begin{vmatrix} -C_{1X2}\,\varepsilon_2 - D\varepsilon_2 + k_3\varepsilon_4 \\ -C_{2X2}\,\varepsilon_2 \\ -C_{3X2}\,\varepsilon_2 + \dot{\varphi}_2 \end{vmatrix} \tag{25}$$

where $\varepsilon_4 = R_{1m} - R_1$ is estimation error of R_1.

Case 1: D constant

In this case on the basis of the Hurvitz stability criterion [18] the following sufficient conditions for stability are obtained (for $\lambda_2 > 0$):

$$C_{1X2} > 0;\; C_2X_2 > 0;\; C_{3X2} < 0 \tag{26}$$

Case 2: D variable

The following sufficient conditions were obtained in this case by the second Liapunov method:

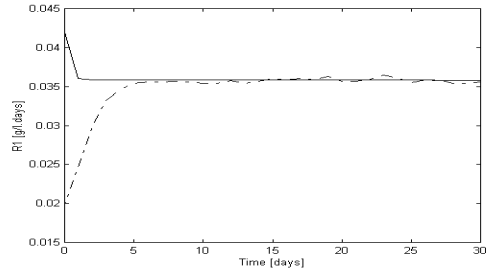
$$\begin{aligned} C_{1X2} &> (C_{3X2}a_4 + C_{2X2}a_5)/a_1 \\ C_{2X2} &= \{a_5(D + \lambda_2 + C_{1X2}) + k_2\lambda_2 a_1\}/a_2 \\ C_{3X2} &= (C_{1X2}a_4 - a_5 - k_2 a_1)/a_3 \end{aligned} \tag{28}$$

where a_1, a_2 and a_3 are positive constants, a_4 and a_5 – negative constants, satisfying the relations:

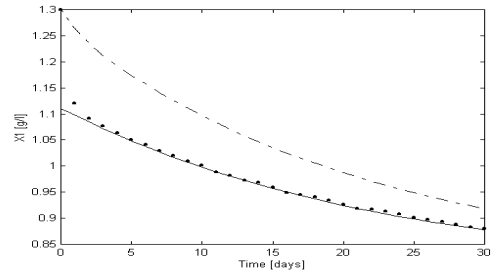
$$a_1a_2 > a_5^2;\; a_1a_2a_3 - a_2a_4^2 - a_3a_5^2 > 0;\; a_2 = a_4k_2\lambda_2 - k_2a_5\,;\; -a_2\,(D+\lambda_2)/k_2\lambda_2 < a_5 \tag{27}$$

Simulation studies, verification and discussion

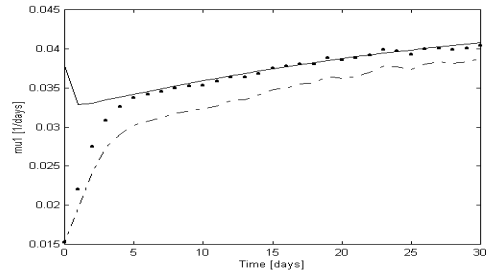
The performance of the proposed estimation algorithms has been investigated by simulations on the process model, described by (1) – (7) with estimated parameters given in Table 1. The values of the design parameters of the proposed estimator and observers have been chosen such that they satisfy the stability conditions. On Fig. 4 (step changes of $S_{20}^{"}$ in the range 25 - 75 g·l^{-1} (D_1 = 0.0375 day^{-1}, D_2 = 0.0125 day^{-1})), Fig. 5 (step changes of D_1 in the range 0.0325 - 0.0625 day^{-1} (D_2 = 0.0125 day^{-1}, $S_{20}^{"}$ = 25 g·l^{-1})) and Fig. 6 (step changes of D_2 in the range 0.0125 - 0.0225 day^{-1} (D_1 = 0.0325 day^{-1}, $S_{20}^{"}$ = 25 g·l^{-1})), the model simulated values of all variables and parameters, i.e., R_1, X_1, μ_1, X_2 and μ_2, are shown on solid lines.



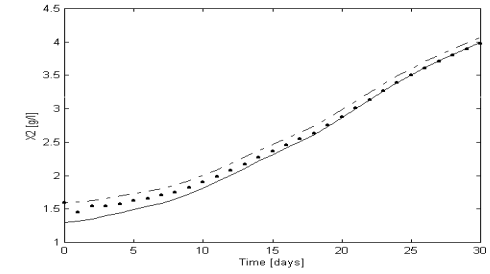
a) R_1 estimates compared with model data



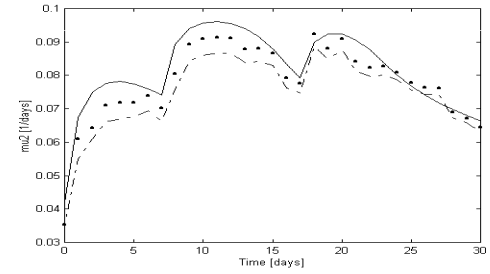
b) Estimates of X_1, obtained by (10) using R_1 estimates and X_1 estimates by observer (14)



c) Estimates of μ_1, obtained by (11) and (15) respectively

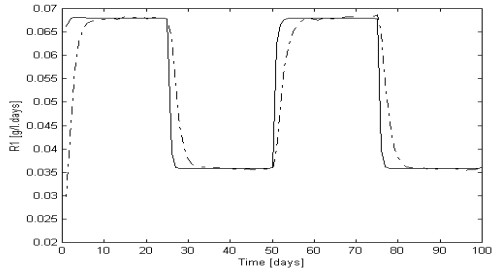


d) Estimates of X_2, obtained by (20) and (24) respectively

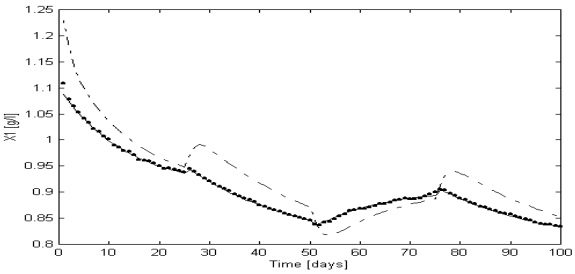


e) Estimates of μ_2, obtained by Eq. (22) and (25) respectively

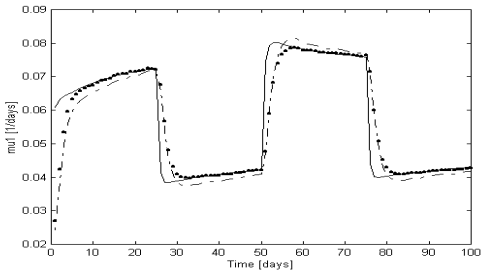
Fig. 4 Step changes of $S_{20}^{''}$ and $h_1 = h_2 = -1$



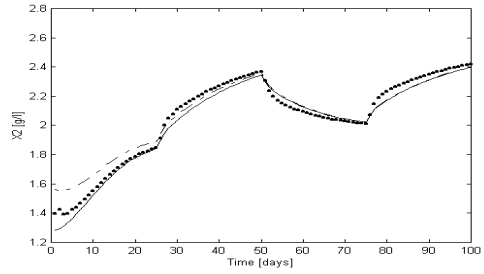
a) R_1 estimates compared with model data



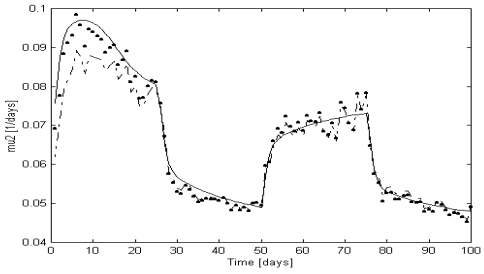
b) Estimates and X_1 estimates by observer (14)



c) Estimates of μ_1, obtained by (11) and (15) respectively

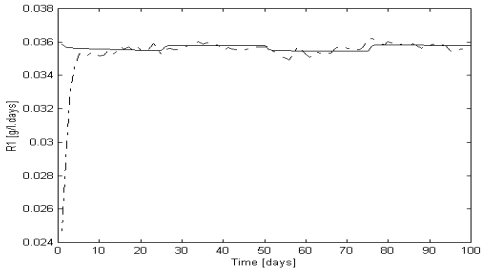


d) Estimates of X_2, obtained by (20) and (24) respectively

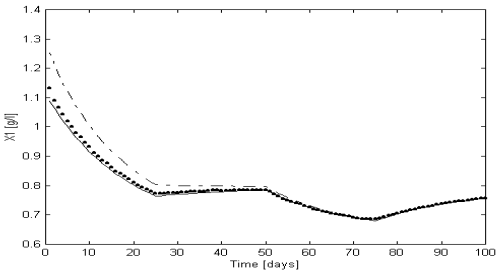


e) Estimates of μ_2, obtained by Eq. (22) and (25) respectively

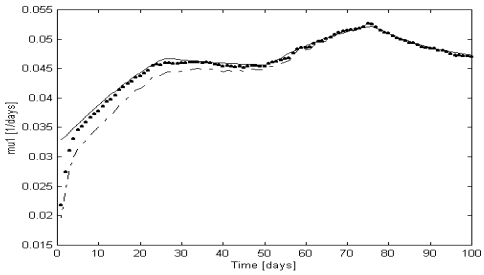
Fig. 5 Step changes of D_1 and $h_1 = h_2 = -1$



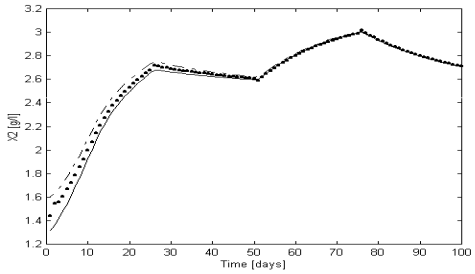
a) R_1 estimates compared with model data



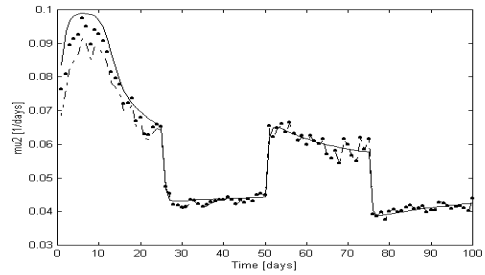
b) Estimates of X_1, obtained by (10) using R_1 estimates and X_1 estimates by observer (14)



c) Estimates of μ_1 , obtained by (11) and (15) respectively

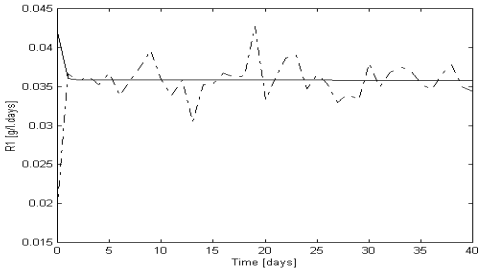


d) Estimates of X_2, obtained by (20) and (24) respectively

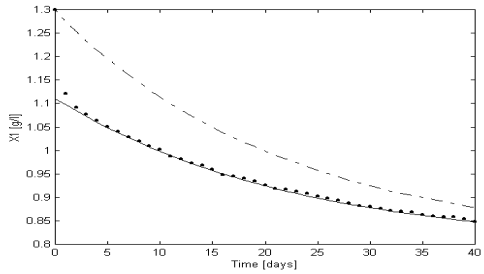


e) Estimates of μ_2, obtained by Eq. (22) and (25) respectively

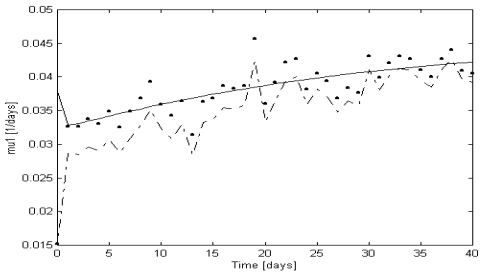
Fig. 6 Step changes of D_2 and $h_1 = h_2 = -1$



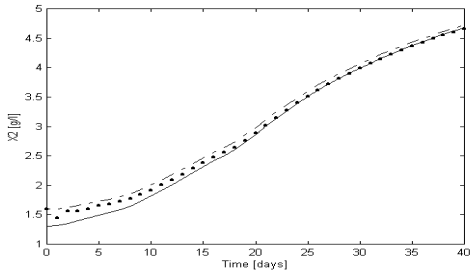
a) R_1 estimates compared with model data



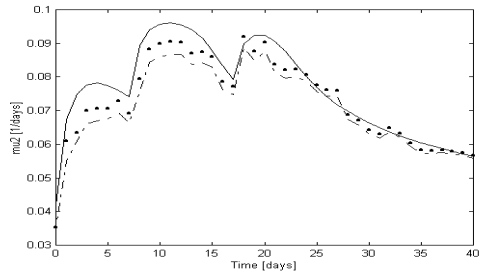
b) Estimates of X_1, obtained by (10) using R_1 estimates and X_1 estimates by observer (14)



c) Estimates of μ_1, obtained by (11) and (15) respectively



d) Estimates of X_2, obtained by (20) and (24) respectively



e) Estimates of μ_2, obtained by Eq. (22) and (25) respectively

Fig. 7 Step changes of $S_{20}^{''}$ and $h_1 = h_2 = -5$

Their estimated values, obtained by R_1 estimator (9), X_1, X_2 observers (14), (24) and relationships (15), (25) under 10% noisy measurements both of S_2 and Q are plotted in dotted line. The estimates of R_1 are obtained by estimator (9) under eigenvalues $h_1 = h_2 = -1$ of the matrix A (12)). The design parameters for the X_1 observer (14) are: $C_{1X1} = 1$; C_{2X1} is calculated according to (18) as a function of D and it is changes between –0.1921 and –0.1983, $C_{3X1} = 0.1$ and $\lambda_1 = 1.4$. These design parameters are calculated using the following values for the parameters a_i: $a_1 = 0.1$, $a_2 = 1$, $a_3 = 3$, $a_4 = -0.0035$, $a_5 = -0.2052$. The design parameters for the X_2 observer (24) are: $C_{1X2} = 1$, C_{2X2} calculated according to (28) as a function of D and it is changes between 0.1258 and 0.136, $C_3X_2 = -1.5$ and $+\lambda_2 = 0.1$. These design parameters are calculated using the following values for the parameters a_i: $a_1 = 0.3678$, $a_2 = 0.294$, $a_3 = 1$, $a_4 = -0.03$, $a_5 = -0.1$. Moreover, the estimations of X_1, X_2, μ_1, and μ_2, given by (10), (20), (11) and (22), respectively, are plotted in dashed lines.

In the above presented results more exact estimates of X_1, μ_1, X_2 and μ_2 are obtained using the proposed X_1 and X_2 observers in comparison with the estimates obtained by indirect estimation of these variables and parameters (time evolution of the variables and parameters of model (1) – (6)). More concretely, X_1 and μ_1 estimates obtained by X_1 observer converge rather quickly (about 5th day changing D_1 and $S_{20}^{"}$ and about 30th day changing D_2 but with very small error) to the true values. Despite that the convergence of estimates of X_2 and μ_2 obtained by X_2 observer is a bit slower, the time of convergence remains considerably smaller in comparison with the indirect estimation.

The same simulations as those presented on Fig. 4, but with $h = h_1 = h_2 = -5$, are presented on Fig. 7. It results in a better convergence speed of the estimators, but to the detriment of the quality of R_1 and μ_1 estimation. The choice of the eigenvalues of the R_1 estimator (9), (20) has then to be related to the level of noise and the type of experimental evaluation (variation of $S_{20}^{"}$, D_2 or D_1). All presented values for C_{iXi} are a good basis for tuning the two observers in the case of practical implementation.

Conclusion

This paper has considered the problem of state and parameter estimation in an AD model. The results are relevant to the future development and the implementation of efficient control strategies, based on addition of acetate or/and glucose containing wastes.

Experimental and analytical studies have shown that addition of acetate or glucose in appropriate quantities allowed improving the biogas production, which is very promising for stabilisation of the AD process both during start-up and process recovering after failure. A simplified model describing the major dynamics, glucose and acetate addition has been proposed based on mass-balance concentrations, for which parameters have been estimated. However those parameters are never exactly known. Indirect estimation of the biomass growth rates has been investigated allowing recovering two specific growth rates and two biomass concentrations. Moreover due to the importance of the above mentioned variables and parameters, a two step approach for their estimation has been proposed using separation of acidogenic stage from the methanogenic phase. In first step, an estimator of R_1 and an observer of X_1 are designed on the basis of mass-balancing equations and on-line measurements of S_2 and Q. An observer of X_2 is developed in the second step, using additionally the estimates of R_1 from the previous step as on-line measurements. The stability

of the proposed estimation algorithms have been proven on the basis of analysis of the error system. The proposed X_1 and X_2 observers have given the possibility to improve the accuracy of the X_1 and X_2 estimates (as well as μ_1 and μ_2 estimates) with respect to these ones obtained from indirect estimation.

Acknowledgements

This work was supported by contract № D 01-376/06 of the Bulgarian National Scientific Fund and by a CNRS – BAS exchange program.

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