15th Triennial World Congress, Barcelona, Spain

TWO-STEP PARAMETER AND STATE ESTIMATION OF THE ANAEROBIC DIGESTION

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Abstract: This paper is devoted to the state and parameter observation for anaerobic digestion process of organic waste. The observation has a two-step structure using separation of acidogenic stage from the methanogenic phase. Two observers and one estimator are built on the basis of a mass-balance nonlinear model of the process, involving a new control input, which reflects the addition of a stimulating substance (acetate). Laboratory experiments have been done with step changes of this new input. The stability of the observers is proven and performances are investigated on experimental data and simulations. *Copyright© 2002 IFAC*

Keywords: anaerobic digestion, lab-scale experiments, acetate supply, non-linear model, parameter and state observation.

1. INTRODUCTION

In the biological anaerobic wastewater treatment processes (methane fermentation) the organic matter is mineralised by microorganisms 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 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. Mathematical modelling represents a very attractive tool for studying this process (Angelidaki, *et al.,* 1999; Bastin and Dochain, 1991), however a lot of models are not appropriate for control purposes due to their complexity. The choice of relatively simple models of this process, their calibration (parameters and initial conditions estimation) and design of software sensors for the unmeasurable variables on the basis of an appropriate model are a very important steps for realization of sophisticated control algorithms (Bastin and Dochain, 1991; Cazzador and Lubenova, 1995; Lubenova, 1999; van Impe, *et al*., 1998).

The aim of this paper is twofold:

-to calibrate the 4^{th} order non-linear model of the methane fermentation with addition of a stimulating substance which may be viewed as control input (influent acetate concentration or acetate flow rate);

-using two measurable process variables to design estimators of the growth rates and observers of the concentrations of the two main groups of microorganisms (acidogenic and methanogenic), appropriate for future control purposes.

2. PROCESS MODELLING

2.1. Experimental Studies

Laboratory experiments hase been carried out in a 3-liter glass vessel CSTR bioreactor with highly concentrated organic pollutants (animal wastes) at mesophillic temperature and addition of acetate in low concentrations (mixed with the effluent organics and pH regulation of the added substrate) (Simeonov and Galabova, 1998). The tank is mechanically stirred by electrical drive and maintained at a constant temperature 34±0.5°C by computer controller. 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^o), redox, speed of agitation (n) and biogas flow rate (Q). The responses of Q are obtained for step changes of the acetate addition. The reported data offer the suggestion that acetate positively affects the methane production (when pH is in the admissible range) and increased levels of acetate as electron donor result in faster rates of methanogenesis.

2.2. Model of the Process

On the basis of the above-presented experimental investigations and following the so-called two-stage biochemical scheme of the methane fermentation (Bastin and Dochain, 1991), the following 4th order non-linear model with two control inputs is proposed (Simeonov and Galabova, 1998):

$$\frac{dX_1}{dt} = (m_1 - D)X_1 \qquad (1)$$

$$\frac{dS_1}{dt} = -k_1 m_1 X_1 + D_1 S_o' - DS_1 \qquad (2)$$

$$\frac{dX_2}{dt} = (m_2 - D)X_2 \qquad (3)$$

$$\frac{dS_2}{dt} = -k_2 m_2 X_2 + k_3 m_1 X_1 + D_2 S_o'' - DS_2 \qquad (4)$$

$$Q = k_4 m_2 X_2 \qquad (5)$$

For the non-linear functions m_1 and m_2 the following structures are adopted:

$$m_1 = \frac{\mu_{max\,1} S_1}{k_{S1} + S_1}; \qquad m_2 = \frac{\mu_{max2} S_2}{k_{S2} + S_2 + S_2^2 / k_{i2}}, \qquad (6)$$

where X [g/l], S[g/l], m[day^{-1}] are the bacteria concentration, the associated substrate concentration and the specific growth rate, respectively and Q[l/day] is the biogas flow rate. Indices 1 and 2 stand for the acidogenic and the methanogenic phases respectively. k_1, k_2, k_3, k_4[l/g], μ_{max1}[day^{-1}], μ_{max2}[day^{-1}], k_{s1}[g/l], k_{s2}[g/l], k_{i2} [g/l] are coefficients, D_1 [day^{-1}] is the dilution rate for the inlet soluble organics with concentration S_0' [g/l], D_2 [day^{-1}] is the dilution rate for the inlet acetate with concentration S_0'' [g/l] and $D=D_1+D_2$ is the total dilution rate.

S_0' is generally an unmeasurable perturbation (on line), while Q and S_2 are measurable outputs, D_1 and D_2 are control inputs and S_0'' is a known constant or control input. In all cases the washout of microorganisms is undesirable, that is why changes of the control input D and the perturbation S_0' are possible only in some admissible ranges (for fixed value of S_0''):

$$0 \le D \le D^{sup}; \quad S_0'^{\,inf} \le S_0' \le S_0'^{\,sup} \qquad (7)$$

2.3. Parameter Identification

A sensitivity analysis with respect to nine coefficients was made only on the basis of simulation studies and they were divided into the following two groups: $k_1 \div k_4$ in the first group, μ_{max1}, μ_{max2}, k_{i2}, k_{s1} and k_{s2} in the second group. Applying the methodology from (Simeonov, 2000) estimation starts with the first (more sensitive) group of coefficients with known initial values of all coefficients using optimisation method; estimation of the second group of coefficients with the above determined values of the first group is the following step, etc. Experimental data were given by measurements of S_2 and Q, with given conditions S_0', S_0'', D_1 and D_2. Results are summarised in Table 1.

Table 1. Values obtained for the coefficients of the 4th order model with acetate addition

μ_{max1}	μ_{max2}	k_{s1}	k_{s2}	k_1	k_2	k_3	k_4	k_{i2}
0.2	0.25	0.3	0.87	6.7	4.2	5	4.35	1.5

Some experimental and simulation results are compared on Fig.1 in the following conditions: D_1 = 0.0375=const., D_2 = 0.0125=const., S_0' =7.5 and S_0'' =25 from t = 0 to 6; S_0'' =50 from t = 7 to 16; S_0'' =75 from t = 17 to 35. Experimental data for D_2=0.0125 with the first step change of S_0'' have served for parameter estimation with initial values of the estimated parameters obtained from other experiment without acetate additation (D_2=0). (Simeonov, 2000). Experimental data for D_2=0.0125 with the 2nd and 3rd step changes of S_0'' were used for model validation. It is evident the behavior of the model with the new control input is satisfying comparing to the process one.

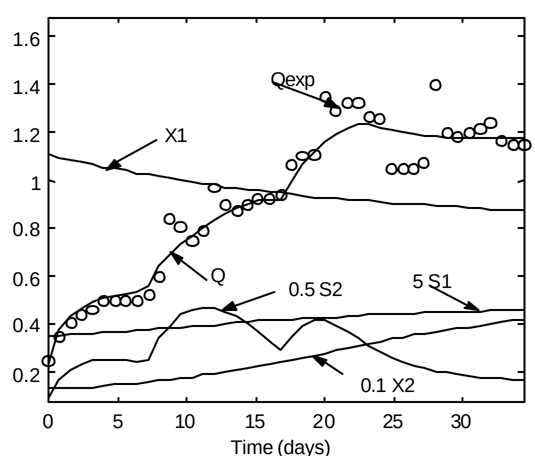

Fig.1. Evolution of X_1, X_2, S_1, S_2, Q and Q_{exp} in the case of step addition of acetate

3. STATE ESTIMATION

3.1. Problem Statement

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

A1. The growth rate $R_1 = m_1 X_1$ associated to acidogenic bacteria, is unknown time-varying parameter, which is 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 substrate 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. The estimation approaches proposed by Bastin and Dochain (1990) cannot be applied for the considered bioprocess.

3.2 Indirect State and Parameter Estimation

The indirect estimation is a simple method for restore of state and parameters, using process models: diferential equations or (and) kinetic models.

3.3. 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:

$$Q_m = Q + e_1; \quad S_{2m} = S_2 + e_2,$$

where e_1 and e_2 are measurements noises.

The following observer-based estimator of R_1 is proposed using the dynamical equation (4) of S_2 concentration:

$$\begin{aligned}\frac{d\hat{S}_2}{dt} &= -DS_{2m} + k_3\hat{R}_1 - k_2 R_{2m} \\ &+ D_2 S_0'' + C_{1R1}(S_{2m} - \hat{S}_2) \\ \frac{d\hat{R}_1}{dt} &= C_{2R1}(S_{2m} - \hat{S}_2)\end{aligned} \quad , \qquad (8)$$

where $R_{2m}=Q_m/k_4 = R_2 + e_1/k_4$ are measured values of R_2, e_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:

$$\dot{\hat{X}}_{1m} = \hat{R}_1 - D\hat{X}_{1m} \qquad (9)$$

where $\hat{R}_1$ is the estimate of R_1 obtained by estimator (8), while the m_1 estimate can be derived on the basis of relationship:

$$\hat{m}_{1m} = \hat{R}_1 / \hat{X}_{1m} \qquad (10)$$

Stability Analysis; Consider the error system associated to the observer (8):

$$\frac{dx}{dt} = Ax + u \qquad (11)$$

$$x = \begin{vmatrix} \tilde{S}_2 \\ \tilde{R}_1 \end{vmatrix} = \begin{vmatrix} S_2 - \hat{S}_2 \\ R_1 - \hat{R}_1 \end{vmatrix}; \quad A = \begin{vmatrix} -C_{1R1} & k_3 \\ -C_{2R1} & 0 \end{vmatrix};$$

$$u = \begin{vmatrix} De_2 + k_2 \dfrac{e_1}{k_4} - C_{1R1} e_2 \\ -C_{1R1} e_2 + \dfrac{dR_1}{dt} \end{vmatrix},$$

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; To improve the convergence rate and consequently the estimation accuracy, a “software sensor” of X_1 is derived. The proposed estimation algorithm can be considered as a modification of the observers proposed in (Dochain, 1986) concerning cases when the estimated variable is not observable from measurements. The dynamics of S_2 (4) is considered and the following auxiliary parameter is defined:

$$j_1 = R_1 + l_1 X_1, \qquad (12)$$

where l_1 is a bounded positive real number. Substituting R_1 from (12) in the dynamical equation of S_2 (4), the following observer of X_1 is derived:

$$\begin{aligned}\frac{d\hat{S}_2}{dt} &= -DS_{2m} + k_3\hat{j}_1 - k_3 l_1 \hat{X}_1 - k_2 R_{2m} + D_2 S_0'' + C_{1X1}(S_{2m} - \hat{S}_2) \\ \frac{d\hat{X}_1}{dt} &= \hat{j}_1 - (D + l_1)\hat{X}_1 + C_{2X1}(S_{2m} - \hat{S}_2) \\ \frac{d\hat{j}_1}{dt} &= C_{3X1}(S_{2m} - \hat{S}_2)\end{aligned} \qquad (13)$$

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

More accurate estimates of the specific growth rate m_1 (in comparison with those derived from (10)) can be obtained using the kinetic model:

$$\hat{m}_1 = \hat{R}_1 / \hat{X}_1, \qquad (14)$$

where $\hat{R}_1$ are the estimates of R_1 obtained from (8), while $\hat{X}_1$ are the estimates of X_1, obtained by observer (13).

Stability Analysis; Consider the dynamics of the estimation error (11). In the considered case, the values of the matrix and vectors are:

$$\mathrm{x} = \begin{vmatrix} \tilde{S}_2 \\ \tilde{X}_1 \\ \tilde{j}_1 \end{vmatrix} \quad \mathrm{A} = \begin{vmatrix} -C_{1X1} & -l_1 k_3 & k_3 \\ -C_{2X1} & -D - l_1 & 1 \\ -C_{3X1} & 0 & 0 \end{vmatrix};$$

$$\mathrm{u} = \begin{vmatrix} -C_{1X1}\, e_2 - De_2 \quad -k_2 e_3 \\ -C_{2X1}\, e_2 \\ -C_{3X1}\, e_2 + \dot{j}_1 \end{vmatrix}, \qquad (15)$$

where $e_3 = R_{2m} - R_2$ is estimation error of R_2.

Since the matrix A, connected with the error system (15) is time-varying through the dilution rate, the stability of the observer (13) has to be proven using method of Lyapunov.

Let the coefficients a_1, a_2, a_3, a_4 be positive numbers, satisfying the following assumptions:

A4. $a_1 a_2 > a_5^2$

A5. $a_1 a_2 a_3 - a_2 a_4^2 - a_3 a_5^2 > 0$

A6. $a_2 = a_4 k_3 \lambda_1 - k_3 a_5$

A7. $-a_2 (D+\lambda_1)/ k_3\lambda_1 < a_5 < a_4 \lambda_1 (D+\lambda_1)/D$

A8. $C_{2X1} = \{ a_1 k_3 \lambda_1 + a_5 (D+\lambda_1 + C_{1X1})\}/ a_2$

A9. $C_{3X1} = (-C_{1X1} a_4 + a_5 + k_3 a_1)/ a_3$

A10. $C_{1X1} > (-C_{3X1} a_4 + C_{2X1} a_5)/a_1$

Lemma 1: Under assumptions A1 to A10, there exist positive finite constants c_0, c_1, c_2 such that the error vector $\mathrm{x} = \begin{vmatrix} \tilde{S}_2 & \tilde{X}_1 & \tilde{j}_1 \end{vmatrix}^T$, is bounded for all t as follows:

$$\|\mathrm{x}(t)\| \le c_0 \|\mathrm{x}(t)\| + c_1 M_1 + c_2 \qquad (16)$$

Proof:

1. First it will be proved that the homogeneous part of the error system (11), (15) is exponentially stable. If $D³0$, we consider the following quadratic function:

$$\mathrm{V}(\tilde{S}_2, \tilde{X}_1, \tilde{j}_1) = 0.5 a_1 \tilde{S}_2^{\,2} + 0.5 a_2 \tilde{X}_1^{\,2} + 0.5 a_3 \tilde{j}_1^{\,2} - a_4 \tilde{j}_1 \tilde{S}_2 - a_5 \tilde{X}_1 \tilde{S}_2 \qquad (17)$$

This function is positive by assumptions A4, A5.

The time derivative of $\mathrm{V}(\tilde{S}_2\ \tilde{X}_1\ \tilde{j}_1)$ is :

$$\begin{aligned} \frac{\mathrm{dV}}{\mathrm{dt}}(\tilde{S}_2, \tilde{X}_1, \tilde{j}_1) &= (-C_{1X1} a_1 + C_{3X1} a_4 + C_{2X1} a_5)\tilde{S}_2^{\,2} \\ &\{-a_2 (D + l_1) + l_1 k_3 a_5\}\tilde{X}_1^{\,2} - k_3 a_4 \tilde{j}_1^{\,2} \\ &\{-l_1 k_3 a_1 + C_{1X1} a_5 + a_5 (D + l_1) - C_{2X1} a_2\}\tilde{X}_1 \tilde{S}_2 \\ &+(k_3 a_1 - C_{3X1} a_3 - a_5 + C_{1X1} a_4)\tilde{j}_1 \tilde{S}_2 \\ &+(a_2 + l_1 k_3 a_4 - a_5 k_3)\tilde{j}_1 X_1 \end{aligned} \qquad (18)$$

Define the function:

$$q(\|\mathrm{x}\|) = (C_{1X1} a_1 - C_{3X1} a_4 - C_{2X1} a_5)\tilde{S}_2^{\,2} \\ \{+a_2 (D_{\min} + l_1) - l_1 k_3 a_5\}\tilde{X}_1^{\,2} + k_3 a_4 \tilde{j}_1^{\,2}$$

where $D_{min} < D < D_{max}$

According the assumptions A6, A7, this function is positive and non-decreasing. Therefore, the exponential stability of the unforced part of the system (15) follows from theorems 9.9-9.11 (Hsu and Meyer, 1972).

2. The forcing term of the error system (11), (15) is bounded in the following way:

$$\mathrm{u} = \begin{vmatrix} -C_{1X1} e_2 - De_2 \quad -k_2 e_3 \\ -C_{2X1} e_2 \\ -C_{3X1} e_2 + \dot{j}_1 \end{vmatrix} < \begin{vmatrix} -C_{1X1} M_2 - DM_2 \quad -k_2 M_3 \\ -C_{2X1} M_2 \\ -C_{3X1} M_2 + M_4 \end{vmatrix} \mathrm{w}$$

here

$|e_2| < M_2$; $|e_3| < M_3$; $|\dot{j}_1| < M_4$

with M_2- M_4 - upper bounds.

3. Then it is a standard results that the state of the system (11), (15) is bounded (Theorem A2.6, (Bastin and Dochain, 1991).

3.4. Estimator and Observer Design for the Methanogenic Stage

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

$$\dot{\hat{X}}_{2m} = R_{2m} - D\hat{X}_{2m}, \qquad (19)$$

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

$$R_{2m} = Q_m/k_4 \qquad (20)$$

The estimation of the specific growth rate m_2 can be realised from the kinetic model:

$$\hat{m}_{2m} = R_{2m} / \hat{X}_{2m} \qquad (21)$$

Similarly to (9), the convergence rate of X_2 estimates to its true values in (19) 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. Analogously to X_1 observer, the structure of this estimation algorithm is derived using the following auxiliary parameter:

$$j_2 = R_2 + l_2 X_2 \quad , \qquad (22)$$

where l_2 is a bounded real number.

By combining (22) and (4), it is possible to propose the following adaptive observer of X_2:

$$\begin{aligned} \frac{d\hat{S}_2}{dt} &= -DS_{2m} - k_2 \hat{j}_2 + k_2 l_2 \hat{X}_2 \\ &+ k_3 R_{1m} + D_2 S_0'' + C_{1X2}(S_{2m} - \hat{S}_2) \\ \frac{d\hat{X}_2}{dt} &= \hat{j}_2 - (D + l_2)\hat{X}_2 + C_{2X2}(S_{2m} - \hat{S}_2) \\ \frac{d\hat{j}_2}{dt} &= C_{3X2}(S_{2m} - \hat{S}_2) \end{aligned} \qquad (23)$$

where C_{1X2}, C_{2X2} C_{3X2} are observer parameters and R_{1m} is the estimate of R_1 obtained by estimator (8).

Like m_1, more accurate estimates of the specific growth rate m_2 (in comparison with those derived from (21)) can be obtained using the kinetic model:

$$\hat{m}_2 = R_{2m} \,/\, \hat{X}_2 , \tag{24}$$

where $\hat{X}_2$ are the estimates of X_2, obtained by (23).

Stability Analysis; This analysis for the observer (23) is similar to the one for observer (13) under the following assumptions:

A11. $a_1\, a_2 > a_5^2$
A12. $a_1\, a_2\, a_3 - a_2\, a_4^2 - a_3\, a_5^2 > 0$
A13. $a_2 = a_4\, k_2\lambda_2 - k_2 a_5$
A14. $-a_2\,(D+\lambda_2)/\, k_2\lambda_2 < a_5 < a_4\, k_2\lambda_2\,(D+\lambda_2)/D$
A15. $C_{2X2} = \{a_5\,(D+\lambda_2 + C_{1X2}) + k_2\lambda_2 a_1\}/\, a_2$
A16. $C_{3X2} = (C_{1X2}\, a_4 - a_5 - k_2 a_1)/\, a_3$
A17. $C_{1X2} > (C_{3X2}\, a_4 + C_{2X2} a_5)/a_1$

where the coefficients a_1, a_2, a_3 a_4 are positive numbers, while a_4 and a_5 - negative numbers.

Lemma 2: Under assumptions A1–A3, A11-A17, there exist positive finite constants l_0, l_1, l_2 such that the error vector $x = \left|\tilde{S}_2 \;\; \tilde{X}_2 \;\; \tilde{j}_2\right|^T$, is bounded for all t as follows:

$$\|x(t)\| \le l_0 \|x(t)\| + l_1 M_1 + l_2 \tag{25}$$

Proof: it is similar to the proof of Lemma 1.

4. SIMULATION STUDIES

The performances of the proposed estimation algorithms are investigated by simulations on a process model, described by (1-7). The values of the design parameters of the proposed estimator and observers are chosen using stability conditions. On Fig. 2 to Fig. 6 are shown in solid lines the true values of R_1, X_1, m_1 and X_2, m_2, respectively, and their estimated values, obtained by R_1 estimator (8), X_1 and X_2 observers (13), (23), (14), (24) and relationships (9), (10), (19), (21) (indirect estimation) under noise free measurements of S_2 and Q and step changing D_1 in the range 0.0325-0.0625.

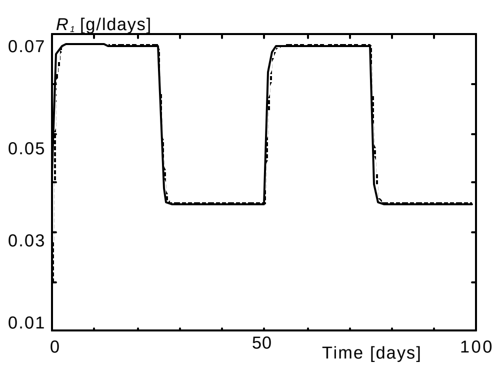

Fig. 2 R_1 estimates under h1=h2= -5 compared with model data.

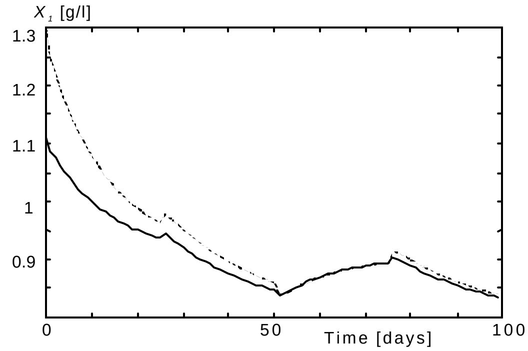

Fig. 3 Estimates of X_1, obtained by (9) using R_1 estimates and X_1 estimates by observer (13)

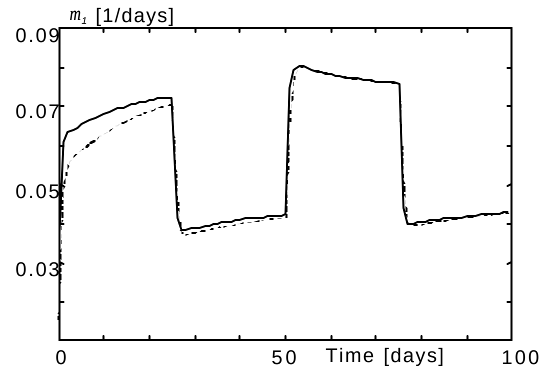

Fig. 4 Estimates of m_1 , obtained by (10) and (14) respectively

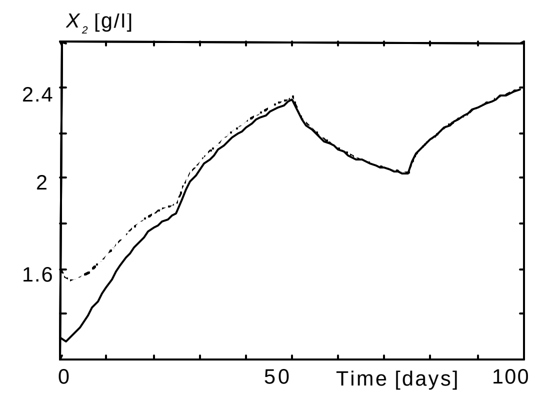

Fig. 5 Estimates of X_2, obtained by (19) and (23) respectively

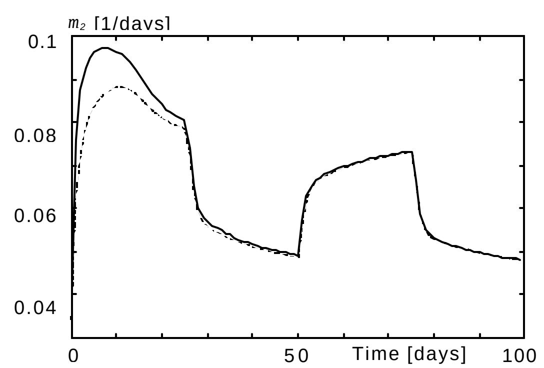

Fig. 6 Estimates of m_2, obtained by equation (21) and (24) respectively

The estimates of R_1 are obtained by estimator (8) with eingenvalues h_1=h_2=-5 of matrix A (11). The estimates of X_1, derived from (9) are plotted with dashed line, while the X_1 estimates by observer (13) (under $C_{1X1}=1$; C_{2X1} calculated according the assumption A8, $C_{3X1}=0.5$ and $+l_1=1.4$) - with dotted line. The estimates of m_1, calculated from (10) and (14) are denoted with dashed and dotted lines respectively. The estimates of X_2, obtained by (19) are plotted with dashed line. The estimates X_2 by observer (23) (with dotted line) are obtained under $C_{1X2}=1$; C_{2X2} calculated according the assumption (A15), C_{3X2}= -1.2 and $+l_2=0.1$. With dashed and dotted lines are marked m_2 estimates by (21) and (24) respectively.

Simulations under 10% noisy measurements both of and are performed. All simulation results confirm the stability of the proposed estimation algorithms.

The simulation investigations show that more exact estimates of X_1, m_1, X_2, m_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.

The estimates of X_1 and m_1 obtained by X_1 observer converge very quicly (about 5th day after changing D_1) to the true values. The dynamic errors connected with the estimation of X_2 and m_2 by X_2 observer are considerably smaller that those obtained by the indirect estimation.

5. CONCLUSION

This paper has considered the problem of state and parameter estimation in an anaerobic digestion process for organic wastes removal and methan production. The result are relevant to the future development and the implementation of efficient control strategies, based on addition of acetate.

Experimental and analytical studies have shown that addition of acetate allowed to improve the biogas production, which is very promising for stabilization of the anaerobic digestion process both during start-up and process recovering after failure. A simplified model describing the major dynamics and acetate addition was 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 to recover 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 X_2 and Q. An observer of X_2 is synthesis in 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 m_1 and m_2 estimates) with respect to these ones obtained from indirect estimation.

Acknowledgements*: This work was supported by contract No TH-1004/00 of The Bulgarian National Found "Scientific researches" and by a CNRS-BAS exchange program.*

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