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DESIGN OF SOFTWARE SENSORS FOR UNMEASURABLE VARIABLES OF ANAEROBIC DIGESTION PROCESSES

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Abstract: The paper deals with software sensor design for unmeasurable variables of anaerobic digestion processes. For this purpose, different mathematical models of anaerobic digestion and different theoretical approaches (differential algebraic approach, Kalman filter modifications and H-infinity filter) have been applied to develop software sensors as dynamic relations between some easily measurable variables and some unmeasurable ones (specific growth rates, biomass and substrate concentrations) of the most important bacteria participating in these processes. Comparative studies have been provided via computer simulations. The experimental validation of the sensors is under investigation on a pilot-scale anaerobic bioreactor with computer monitoring system.

Key words: Anaerobic digestion, software sensor, algebraic system theory, Kalman filter, H-infinity filter

Резюме: Статията разглежда проектиране на софтуерни сензори за неизмерими променливи на анаеробното разграждане на органични отпадъци. За тази цел различни математически модели на анаеробно разграждане и различни теоретични подходи (диференциално-алгебричен подход, филтър на Калман и H-безкрайност филтър) са приложени за разработване на софтуерни сензори като динамични връзки между някои лесно измерими променливи и някои неизмерими (специфични скорости на растеж, концентрации на биомаса и на субстрат) за най-важните групи бактерии, участващи в процеса. Представени са сравнителни изследвания чрез компютърни симулации. Експерименталното валидиране на сензорите е в процес на изследване на пилотен анаеробен биореактор с компютърна система за мониторинг.

Ключови думи: анаеробно разграждане, софтуерни сензори, теория на алгебричните системи, филтър на Калман, H-безкрайност филтър

1. INTRODUCTION

Anaerobic digestion (AD) is a biotechnological process widely used in life sciences and a promising method for solving some energy and ecological problems in agriculture and agro-industry. In such kind of processes, generally carried out in continuously stirred tank bioreactors (CSTR), the organic matter is depolluted by microorganisms into biogas (consisting mainly of methane and carbon dioxide) and digestate (potential manure) in the absence of oxygen (Deublein and Steinhauser, 2008). The biogas is an additional energy source which can replace fossil fuel sources. It therefore has a direct positive effect on greenhouse gas reduction.

Unfortunately this process is very complex and can be unstable, particularly at changes in the environment, for example following an increase in influent concentration (Ward et al., 2008) or in dilution rate (Converti et al., 2008), or a change in the nature of the feedstock.

An active research problem is to better understand the dynamics of growth and death of the different populations of the complex community of bacteria acting during AD processes. However, it is practically impossible to measure on-line different bacterial concentrations or specific growth rates (Deublein and Steinhauser, 2008). Other biochemical variables important for the AD processes are too expensive to be measured. In practice, only biogas flow rate can be easily measured on-line. One of the most promising ways to solve this problem is the design of software sensors for estimating some biochemical variables on the basis of an AD mathematical model and some easily measured process parameters (Dochain and Vanrolleghem, 2001; Lubenova et al., 2002; Ward et al., 2011). A software sensor is a combination of hardware sensors and an internal software estimator, which predicts parameters that require expensive equipment or cannot be measured directly. The realization of software sensors is a preferable method of continuous monitoring of some key process variables and of using this information to make decisions regarding the digester loading, either through automatic organic loading rate systems or advice to operators. This has economic sense in terms of reduced capital costs and improved biogas output.

Software sensors have been used in practice to monitor anaerobic digestion processes (Ward et al., 2008). So far, there have been no published software sensors of different bacterial concentrations or specific growth rates with respect to biogas flow rate, methane and carbon dioxide levels in the biogas. Such software sensors are important not only for gaining insight into and testing biochemical theories

for interactions between different populations of the complex community of bacteria acting during AD processes, but also for optimizing methane production.

The aim of this paper is to present some recent achievements of our team in the field of software sensor design for unmeasurable variables of AD processes. For this purpose, different mathematical models of AD and different theoretical approaches (differential algebraic approach, Kalman filter modifications and H-infinity filter) have been applied to develop software sensors as dynamic relations between some easily measured variables and some unmeasurable ones (specific growth rates, biomass and substrate concentrations) of the most important bacteria participating in AD processes.

2. PROCESS MODELS

2.1. One-stage model

Consider the continuous AD state-space model presented in (Simeonov, 1999):

$$\begin{aligned} \frac{dX}{dt} &= (\mu - D)X \\ \frac{dS}{dt} &= -K_1\mu X + D(S_{in} - S) \\ Q &= K_2\mu X \end{aligned} \tag{1}$$

where $(X\ S)^T$ is the state vector of the concentrations [g/L] of: biomass – X, and substrate – S; D is the control input – dilution rate [day^{-1}]; Q is the output – biogas flow rate [L/day]; constant parameters: K_1 and K_2 are yield coefficients; S_{in} is the input substrate concentration [g/L]; the variable parameter μ is the specific growth rate of bacteria [day^{-1}] assumed to be of Monod type:

$$\mu = \frac{\mu_m S}{k_s + S} \tag{2}$$

where μ_m, and k_s and are kinetic coefficients.

2.2. Three-stage model

In (Hill and Barth, 1977) hydrolysis (enzymatic degradation of insoluble organics to soluble organics), acidogenesis (transformation of the soluble organics to acetate) and methanogenesis

(transformation of the acetate to methane) are considered, developing a model for AD of cattle manure as follows:

$$\frac{dS_0}{dt} = -DS_0 - \beta X_1 S_0 + DY_p.S_{in} \tag{3}$$

$$\frac{dX_1}{dt} = (\mu_1 - D).X_1 \tag{4}$$

$$\frac{dS_1}{dt} = -DS_1 + \beta X_1 S_0 - \mu_1 \frac{X_1}{Y_1} \tag{5}$$

$$\frac{dX_2}{dt} = (\mu_2 - D).X_2, \tag{6}$$

$$\frac{dS_2}{dt} = -DS_2 + Y_b \mu_1 X_1 - \mu_2 \frac{X_2}{Y_2}, \tag{7}$$

$$Q = Y_g \mu_2 X_2 \tag{8}$$

where: X_1 and X_2 [g/L] are concentrations of acidogenic (with specific growth rate μ_1 [day^{-1}]) and methanogenic (with specific growth rate μ_2 [day^{-1}]) bacteria, respectively; S_1 [g/L] – soluble carbohydrate concentration; S_2 [g/L] - acetate concentration; Q [L/day] - biogas flow rate; D [day $^{-1}$] – dilution rate. The first equation of the model (3) describes the hydrolysis of cattle manure with concentration S_{in} resulting in soluble organics with concentration S_0 (β and Y_p are coefficients of appropriate dimensions). Equations (4) and (5) describe the acidogenic step, equations (6) and (7) describe the methanogenic step. Equation (8) describes the biogas output. In this model Y_1, Y_2, Y_b and Y_g are yield coefficients of appropriate dimensions, μ_1 and μ_2 are with Monod form:

$$\mu_1 = \frac{\mu_{\max 1}.S_1}{(k_{s1} + S_1)}, \quad \mu_2 = \frac{\mu_{\max 2}.S_2}{(k_{s2} + S_2)} \tag{9}$$

where μ_{max1}, μ_{max2}, and k_{s1}, k_{s2} are kinetic coefficients .

2.3. Five-stage model

This model includes the formation of methane (about 30%) by the hydrogenotrophic methanogenic bacteria (Karakashev et al., 2004):

$$\begin{cases} \dfrac{dS_0}{dt} = -\beta \dfrac{S_0 X_1}{S_2 + K_{i,acet}} + DY_e S_{in} - DS_0 \\ \dfrac{dX_1}{dt} = \mu_1 X_1 - DX_1 \\ \dfrac{dS_1}{dt} = \beta \dfrac{S_0 X_1}{S_2 + K_{i,acet}} - Y_{glu/X_1} \mu_1 X_1 - DS_1 \\ \dfrac{dX_2}{dt} = \mu_2 X_2 - DX_2 \\ \dfrac{dS_2}{dt} = Y_{acet/X_1} \mu_1 X_1 - Y_{acet/X_2} \mu_2 X_2 - Y_{acet/X_3} \mu_3 X_3 - DS_2 \\ \dfrac{dX_3}{dt} = \mu_3 X_3 - DX_3 \\ \dfrac{dS_3}{dt} = Y_{H_2/X_1} \mu_1 X_1 + Y_{H_2/X_3} \mu_3 X_3 - Y_{H_2/X_4} \mu_4 X_4 - K_{H_2} S_3 - DS_3 \\ \dfrac{dX_4}{dt} = \mu_4 X_4 - DX_4 \\ \dfrac{dS_4}{dt} = Y_{CO_2/X_1} \mu_1 X_1 + Y_{CO_2/X_2} \mu_2 X_2 + Y_{CO_2/X_3} \mu_3 X_3 - Y_{CO_2/X_4} \mu_4 X_4 - K_{CO_2} S_4 - DS_4 \\ Q = Y_{CH_4/X_2} \mu_2 X_2 + Y_{CH_4/X_4} \mu_4 X_4 + K_{CO_2} S_4 \end{cases} \tag{10}$$

where X_1, X_2, X_3 and X_4 [g/L] are the concentrations of acidogenic, acetogenic, hydrogenotrophic methanogenic and acetoclastic methanogenic bacteria, respectively; μ_1, μ_2, μ_3 and μ_4 [day^{-1}] are the respective specific growth rates; S_0 [g/L] is the concentration of soluble organics; S_1, S_2, S_3 and S_4 [g/L] are the concentrations of substrates for acidogenic, acetogenic, hydrogenotrophic methanogenic and acetoclastic methanogenic bacteria, respectively; S_{in} [g/L] is the influent concentration of organic matter; Q [L/day] is biogas production rate; D [day^{-1}] is the dilution rate; β, $K_{i,acet}$, K_{H2} , K_{CO2} and Y_e are coefficients of appropriate dimensions; $Y_{glu/X1}$, $Y_{acet/X1}$, $Y_{acet/X2}$, $Y_{acet/X3}$, $Y_{H2/X1}$, $Y_{H2/X3}$, $Y_{H2/X4}$, $Y_{CO2/X1}$, $Y_{CO2/X2}$, $Y_{CO2/X3}$, $Y_{CO2/X4}$, $Y_{CH4/X2}$ and $Y_{CH4/X4}$ are yield coefficients.

2.4. Technological constraints

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

$$0 < D \leq D_{sup};\ S_{in}^{min} \leq S_{in} \leq S_{in}^{max} \tag{11}$$

3. SOFTWARE SENSOR DESIGN VIA THE DIFFERENTIAL ALGEBRAIC APPROACH

3.1. Sensors based on the one-stage model

The specific growth rate of bacteria μ is a quite complex function of the process variables. It is standard to approximate μ by an empirical function of X and S. The choice of such a model usually is difficult and is done on the basis of an expert's knowledge. That is why μ is preferably assumed to be unknown and to be reconstructed via estimation techniques.

Biomass specific growth rate μ is estimated by the following dynamics using online measurements of D and Q (Diop and Simeonov, 2009):

$$\begin{cases} \dot{z} = -Dz + Q \\ \hat{\mu} = \dfrac{Q}{z} \end{cases} \tag{12}$$

where $z = \dfrac{Q}{\mu}$.

The dynamics (12) represents a very simple software sensor for monitoring the specific growth rate of bacteria μ.

3.2. Sensors based on the three-stage model with measurements of D, Q and S_2

3.2.1. <u>Estimation of growth rates</u>

The following estimation scheme for μ_2 was obtained (Diop et al., 2006):

$$\begin{cases} \dot{z}_2 = -Dz_2 + Q \\ \hat{\mu}_2 = \dfrac{Q}{z_2} \end{cases} \tag{13}$$

It yields the following estimation scheme for μ_1:

$$\begin{cases} \dot{z}_1 = -Dz_1 + Q + Y_2 Y_g D S_2 + Y_2 Y_g \hat{\dot{S}}_2 \\ \hat{\mu}_1 = \dfrac{Q + Y_2 Y_g D S_2 + Y_2 Y_g \hat{\dot{S}}_2}{z_1} \end{cases} \tag{14}$$

The dynamics (13) and (14) represent relatively simple software sensors for monitoring the specific growth rates of methanogenic and acidogenic bacteria respectively.

3.2.2. Estimation of biomass concentrations

Assuming μ_1 and μ_2 thus estimated, X_1 and X_2 can be estimated as follows:

$$\begin{cases} \hat{X}_1 = \dfrac{Q + Y_2 Y_g D S_2 + Y_2 Y_g \hat{\dot{S}}_2}{Y_2 Y_b Y_g \hat{\mu}_1} = \dfrac{z_1}{Y_2 Y_b Y_g} \\ \hat{X}_2 = \dfrac{Q}{Y_g \hat{\mu}_2} = \dfrac{z_2}{Y_g} \end{cases} \tag{15}$$

The dynamics (15) represents relatively simple software sensors for monitoring the concentrations of acidogenic (X_1) and methanogenic (X_2) bacteria respectively.

These results are described in details in (Diop et al., 2006).

3.3. Sensors based on the five-stage model with measurements of D, Q, S_2, S_3 and S_4

3.3.1. Observability with respect to D, Q, S_2, S_3 and S_4

Not only yield coefficients are all assumed constant and known but organic substrate concentrations S_2, S_3 and S_4 are also supposed to be measured online. The soluble organics concentration S_0 and the substrate concentration S_1 are not assumed measured.

The observability of biomass specific growth rates μ_1, μ_2, μ_3 and μ_4 with respect to the yield coefficients and S_2, S_3 and S_4 result in differential polynomials of the following form for specific growth rates (Chorukova et al., 2007):

$$\dot{\mu}_i + \mu_i^2 + f_i\,\mu_i = 0,\ \mathrm{i} = 1,2,3,4$$

where the f_i are functions of S_2, S_3, S_4 and their derivatives, D and Q.

This partial result lets think that specific growth rates are again not observable with respect to measured variables.

3.3.2. Estimation with respect to D, Q, S_2, S_3 and S_4

For the five-stage model in the absence of specific growth rate estimation schemes with respect to easily measured variables, one of the last resorts is to identify specific growth rates as functions of the S_i's and X_i's. Biomass concentrations may be estimated based upon these empirical models. Specific growth rates may be empirically identified as follows (Karakashev et al., 2004):

$$\begin{cases} \mu_1 = \mu_{1\max} \dfrac{S_1}{K_{S_1} + S_1} \\ \mu_2 = \mu_{2\max} \dfrac{K_{i,NH_4^+}}{K_{i,NH_4^+} + S_{NH_4^+}} \dfrac{S_2}{K_m X_2 + S_2} \\ \mu_3 = \mu_{3\max} \dfrac{S_2}{K_{S_3} + S_2} \\ \mu_4 = \mu_{4\max} \dfrac{S_3}{K_{S_4} + S_3} \dfrac{S_4}{K_{S_4} + S_4} \end{cases}$$

The software sensors of biomass concentrations and substrate concentration S_0 are as follows:

$$
\begin{cases}
\hat{X}_1 = \dfrac{b_1}{a\mu_1} \\
\hat{X}_2 = \dfrac{b_2 S_2}{\mu_{2\max} \dfrac{K_{i,NH_4^+}}{K_{i,NH_4^+} + S_{NH_4^+}} a S_2 - K_m b_2} \\
\hat{X}_3 = \dfrac{b_3}{a\mu_3} \\
\hat{X}_4 = \dfrac{b_4}{a\mu_4} \\
\hat{S}_0 = \dfrac{\left(\dot{S}_1 + DS_1 + Y_{glu/X_1}\mu_1 X_1\right)\left(S_1 + K_{i,acet}\right)}{\beta \hat{X}_1}
\end{cases}
\tag{16}
$$

where: $b_i = c_{i1}Q + c_{i2}DS_2 + \left(c_{i3} + c_{i4}D\right)S_3 + \left(c_{i5} + c_{i6}D\right)S_4 + c_{i7}\dot{S}_2 + c_{i8}\dot{S}_3 + c_{i9}\dot{S}_4 \quad i = 1, 2, 3 \; or \; 4$

The quantity a and the $c_{i\,j}$'s are functions of the process constant parameters only. It is also noticeable that the b_i's depend on the supposedly measured variables: D, Q, S_2, S_3 and S_4, only.

These results are described in details in (Chorukova et al., 2007).

3.4. Sensors based on the three-stage model with measurements of D, Q, Q_{CH4} and Q_{CO2}

3.4.1. Gas phase modelling

In our case for the overall gas output (biogas) the following equation has been adopted:

$$
Q = Q_{CH4} + Q_{CO2}, \tag{17}
$$

with the following expressions for methane (Q_{CH4}) and carbon dioxide (Q_{CO2}) flow rates:

$$
\begin{aligned}
Q_{CH_4} &= K_{X2CH4}\mu_2 X_2 \\
Q_{CO_2} &= K_{X1CO2}\mu_1 X_1 + K_{X2CO2}\mu_2 . X_2
\end{aligned}
\tag{18}
$$

3.4.2. Estimation of the specific growth rate of bacteria

The analysis of observability of μ_1 and μ_2 with respect to D, Q_{CH4}, Q_{CO2} and all parameters (these are supposed to be constant and known), using the differential algebraic approach, yields the following two systems of differential equations:

$$\dot{\hat{z}}_1 = -(D + k_1)\hat{z}_1 + q_{CO_2} \tag{19}$$

$$\hat{\mu}_1 = \frac{q_{CO_2}}{\hat{z}_1}$$

$$\dot{\hat{z}}_2 = -(D + k_2)\hat{z}_2 + Q_{CH_4} \tag{20}$$

$$\hat{\mu}_2 = \frac{Q_{CH_4}}{\hat{z}_2}$$

where: $q_{CO2} = K_{X_2CH_4} Q_{CO_2} - K_{X_2CO_2}.\mathrm{Q}_{CH_4}$

The quantity q_{CO2} is non-negative since, as given in equations (8) it evaluates to:

$$q_{CO2} = K_{X_2CH_4} K_{X_2CO_2}.\mu_1 X_1 \tag{21}$$

The previous two systems of differential equations (19) and (20) provide software sensors for the specific growth rates of acidogenic and methanogenic bacteria respectively.

3.4.3. Estimation of the acidogenic and methanogenic bacterial concentrations

Applying the same approach for estimation of the acidogenic and methanogenic bacterial concentrations in the anaerobic bioreactor, the following software sensors have been obtained:

$$\hat{X}_1 = \frac{z_1}{K_{X_1CO_2} K_{X_2CH_4}} \tag{22}$$

$$\hat{X}_2 = \frac{z_2}{K_{X_2CH_4}} \tag{23}$$

where expression (22) refers to acidogenic and (23) to methanogenic bacterial concentration.

It is quite evident that only the specific growth rate of methanogenic bacteria $\hat{\mu}_2$ does not depend on the adopted, for the software sensor design, model parameters.

3.5. Experimental studies

3.5.1. Pilot plant with computer monitoring system

Experimental studies of AD of cattle manure have been performed in a pilot-scale anaerobic BR with full volume of 100 L at mesophilic temperature (34^0C). During the experiments different analyses have been done. However, for this study only biogas yield and biogas composition (relative content of CH_4 and CO_2 in the biogas using a Dreger device with infrared sensors) have been measured.

3.5.2. Experimental results

The pilot anaerobic BR with working volume of 80 L has operated in continuous mode with cattle manure and different values of dilution rate (D) and of the concentration of inlet organic matter (S_{in}). A very particular experiment (pulses of the organic load) has been designed including changes of D and S_{in} as shown on Table 1.

Table 1. Changes of D and S_{in} during the experiment

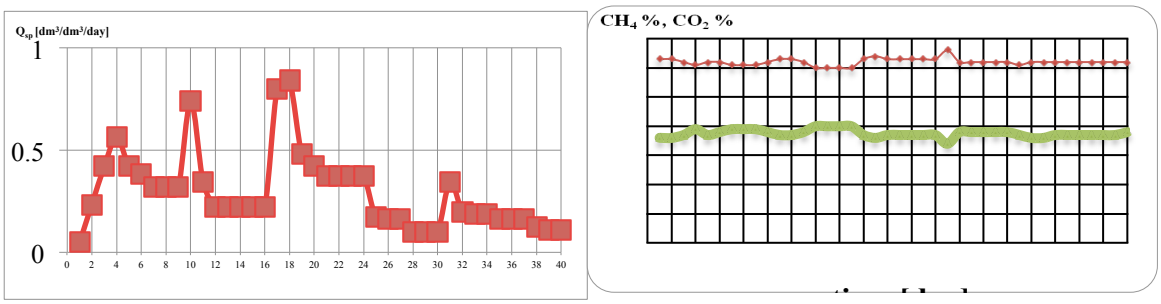
Time [days]	D [day^{-1}]	S_{in} [g/L]
0	0.01	69
1	$Pulse_1 = 0.025$	69
9	$Pulse_2 = 0.02$	69
16	$Pulse_3 = 0.0225$	86
30	$Pulse_4 = 0.025$	40

Some experimental data are presented on Fig. 1 a) and b). On Fig. 1 a) the specific biogas flow rate Q_{sp} evolution for changes of D and S_{in} as shown on Table 1 is presented. The daily biogas flow rate per 1 L of the working volume of the BR has been denoted by Q_{sp}.

On Fig. 1 b) biogas contents evolution (Q_{CH4} *and* Q_{CO2}) for changes of D and S_{in} as shown on Table 1 is presented.

From Fig. 1 a) one may conclude that the evolution of Q_{sp} reflects the above depicted changes of D and S_{in} in an appropriate way.

From Fig. 1 b) one may conclude that the evolution of Q_{CH4} *and* Q_{CO2} in the biogas is not influenced by the above depicted changes of D and S_{in}.



a) b)

Fig. 1. Specific biogas flow rate Q_{sp} evolution (a) and biogas content evolution (Q_{CH4} *and* Q_{CO2}) (b) for changes of D and S_{in} as shown on Table 2.

3.6. Simulation studies

For testing the above obtained software sensors it has been supposed that μ_1 and μ_2 in the model are with Monod form (9).

The model simulation and the processed experimental data (better reflecting the daily changes of Q_{sp}) of Fig. 1a are shown on Fig. 2. Refer to Table 2 for a list of parameter values.

Simulations have been performed with pulse changes of D and step changes of S_{in} as in the pilot experiment conditions (see Table 1). For initialization of the software sensors a 20- day displacement of time, as shown on Fig. 3, has been applied.

Simulation results with software sensors designed for μ_1 and μ_2 are shown on Fig. 4 and 5.

Table 2. Simulation coefficient values

Coefficient	Value	Units
β	4.0	day^{-1}
Y_p	0.144	-
Y_1	0.0546	-
Y_2	0.26	-
Y_b	5.0	-
Y_g	3.1	?
μ_{max1}	0.4	day^{-1}
μ_{max2}	0.25	day^{-1}
k_{s1}	1.9	g/L
k_{s2}	0.37	g/L
k_1	0.04	day^{-1}
k_2	0.025	day^{-1}
K_{X_2CH4}	3.0	3.0
K_{X_1CO2}	0.4	0.4
K_{X_2CO2}	0.6	0.6

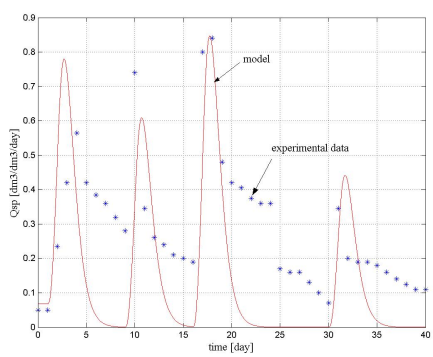


Fig. 2. Estimation validation with pilot-scale data

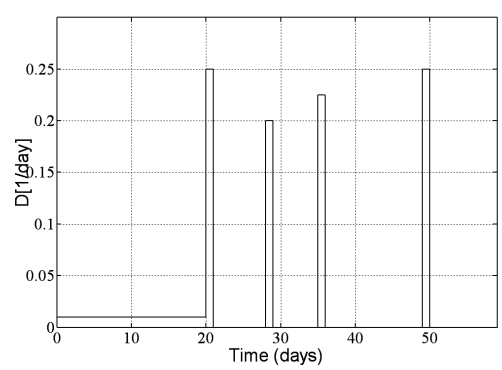


Fig.3. Pulse changes of *D* for simulation purposes

Simulations with software sensors for estimating specific growth rates μ_1 and μ_2 agree with the data obtained with the model. However, the results obtained with software sensors for estimating the concentrations of acidogenic and methanogenic bacteria at this first stage were poor. That is why an investigation of the dynamics of these sensors has been performed with noisy measurement of Q, Q_{CH4} *and* Q_{CO2}(addition of white noise with amplitude of 10 % of the model values), pulse changes of D and step changes of S_{in}, as shown on Table 3.

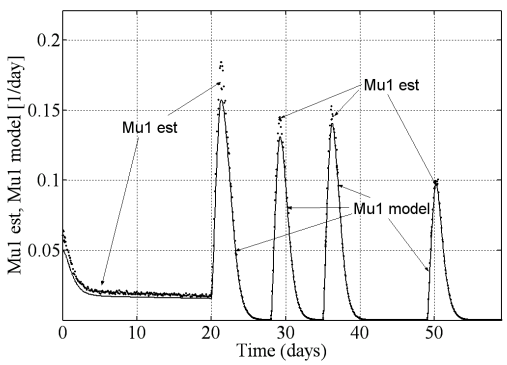


Fig. 4. Simulation results with software sensors for μ_1

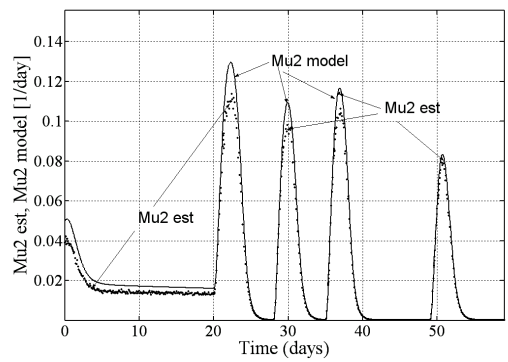


Fig. 5. Simulation results with software sensors for μ_2

For pulse changes of D and step changes of S_{in}, as shown on Table 3, the noisy measurements of Q_{CH4} *and* Q_{CO2} are shown on Fig. 6.

Table 3. Changes of D and S_{in} during the investigation of the software sensor dynamics

t [days]	D [day^{-1}]	S_{in} [g/L]
0	0.025	70
220	0.05	70
300	0.05	50

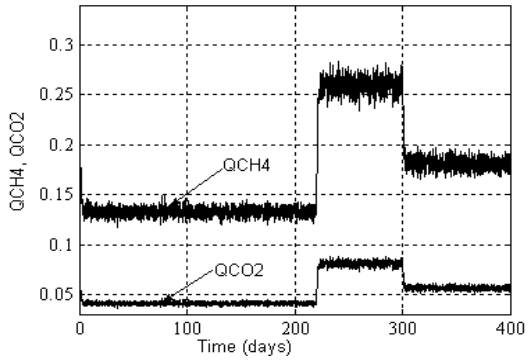


Fig.6. Noisy measurements of Q_{CH4} *and* Q_{CO2} for pulse changes of D and step changes of S_{in}, as show on Table 4.

Simulation results with software sensors designed for estimating μ_1, μ_2, X_1 and X_2 are shown on Figs. 7 – 10 with noisy measurement of Q, pulse changes of D and step changes of S_{in}, as shown on Table 3.

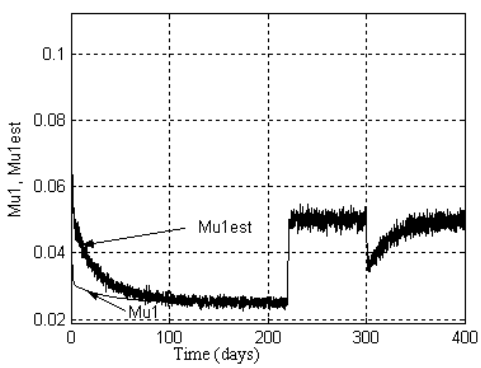


Fig.7. Simulation results with software sensors for μ_1

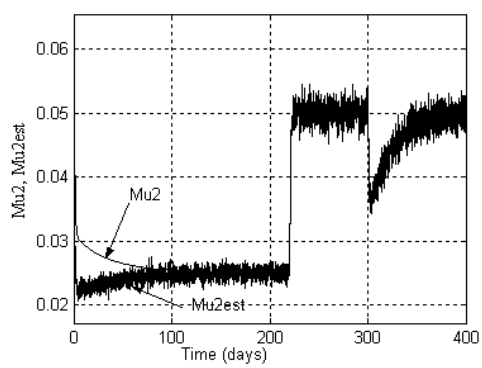
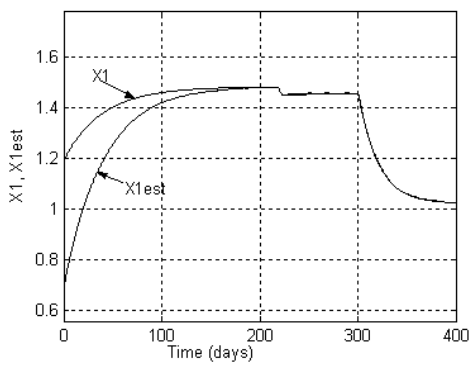


Fig.8. Simulation results with software sensors for μ_2



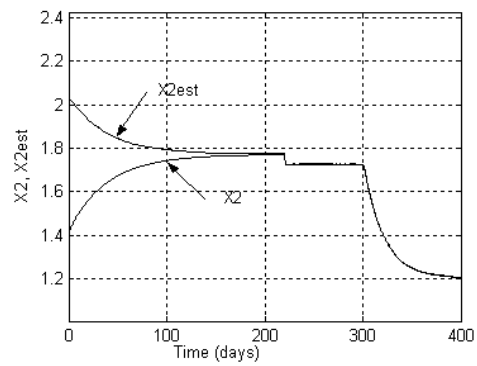


Fig.9. Simulation results with software sensors for X_1

Fig.10. Simulation results with software sensors for X_2

4. SOFTWARE SENSOR DESIGN BASED ON THE ONE-STAGE MODEL VIA KALMAN FILTER

The proposed software sensors reconstruct the unmeasurable variables X and S as time functions, given the measurable output Q under the presence of random perturbations – an internal perturbation $w(t)$ and a measurement noise $v(t)$ for Q, as well as of simultaneous stepwise parameter perturbations.

4.1. Classical Kalman filter

The Kalman filter (KF) (Solodov, 1976) providing optimal mean-square estimate $\hat{Y}$ of the state vector of the linearized process model $Y=[X-X_0 \;\; S-S_0]^T$ (with "T" denoting transpose; X_0 and S_0 being the nominal state trajectories in the neighbourhood of which the model is linearized) is:

$$\frac{d\hat{Y}}{dt} = (A - KC)\hat{Y} + K(Q - Q_0), \quad \hat{Y}(0) = 0 \tag{24}$$

where: A, C are respectively the state and observation matrices of the linearized process model described in (Kalchev et al., 2011);

$$Q_0 = k_2 \mu(S_0) X_0;$$

$$K = \frac{1}{r} P C^T$$

is the filter gain matrix, and the error covariance matrix P is obtained from the Riccati matrix differential equation:

$$\frac{dP}{dt} = AP - \frac{1}{r}PC^TCP + PA^T + BNB^T, \quad P(0) > 0$$

where: B is the control matrix of the linearized process model; r is the covariance parameter of the zero-mean Gaussian white noise modeling the measurement noise *v(t)* as in (Kalchev et al., 2011); $N = diag(q_1, q_2)$ with q_1 and q_2 being the covariance parameters of the respective zero-mean Gaussian white noises modeling the two-component internal perturbation *w(t)* as in (Kalchev et al., 2011).

The dynamics (24) represents a software sensor for monitoring the unmeasurable variables X and S.

4.2. Extended Kalman filter

An Extended Kalman Filter (EKF), corresponding to the classical KF described above, has been developed. Since EKF is based on the nonlinear model, the random internal perturbation w(t) is one-component in this software sensor. The EKF structure may be presented as follows:

$$\begin{aligned} \frac{d(\hat{X} - X_0)}{dt} &= -D_0(\hat{X} - X_0) + \frac{1}{k_2}(\hat{Q} - Q_0) + L_1(Q - \hat{Q}) \\ \frac{d(\hat{S} - S_0)}{dt} &= -D_0(\hat{S} - S_0) - \frac{k_1}{k_2}(\hat{Q} - Q_0) + L_2(Q - \hat{Q}), \end{aligned} \tag{25}$$

where:

$$\hat{Q} = k_2\hat{\mu}\hat{X}, \quad \hat{\mu} = \frac{\mu_m\hat{S}}{k_s + \hat{S}}, \tag{26}$$

L is the filter gain matrix calculated as the matrix P for the classical KF.

The dynamics (25) represents a software sensor for monitoring the unmeasurable variables X and S.

4.3. Deterministic software sensor based on EKF

A deterministic nonlinear software sensor on the basis of EKF theory according to the method in (Johansson, Medvedev, 2003) has been designed. The structure of this software sensor of variables X and S has been presented in (Kalchev et al., 2009) as follows:

$$\begin{aligned} \frac{d\hat{X}}{dt} &= -D\hat{X} + k_2\hat{\mu}(Q-\hat{Q}) + \frac{1}{k_2}Q \\ \frac{d\hat{S}}{dt} &= D(S_{in}-\hat{S}) + \frac{k_2 k_S \mu_m}{(K_S+\hat{S})^2}\hat{X}(Q-\hat{Q}) - \frac{k_1}{k_2}Q \end{aligned} \tag{27}$$

where $\hat{Q}$ and $\hat{\mu}$ are as in (26).

4.4. Simulation studies

4.4.1. <u>Performance analysis at random perturbations</u>

Comparative simulations studies have been performed, concerning the classical KF (24), EKF (25), the differential algebraic software sensor (12) and the classical adjustable software sensor in (Simeonov et al., 1997).

The simulation results obtained with EKF do not differ significantly from those obtained with the classical KF, as the latter one is based on a linearized model in a close neighbourhood of the control action D_0. An exemplary result for the estimation of μ can be seen on Fig. 11.

A selected result from the performance analysis is presented on Fig. 12, concerning the relative error in the estimation of μ by the KF and the classical adjustable software sensor, and on Fig. 13, concerning the average relative error up to the current simulation time in the same estimation. On both figures the KF exhibits smaller errors after the initial convergence period. In this case the maximum relative error of the KF is about 30%, whereas of the other software sensor – about 80%.

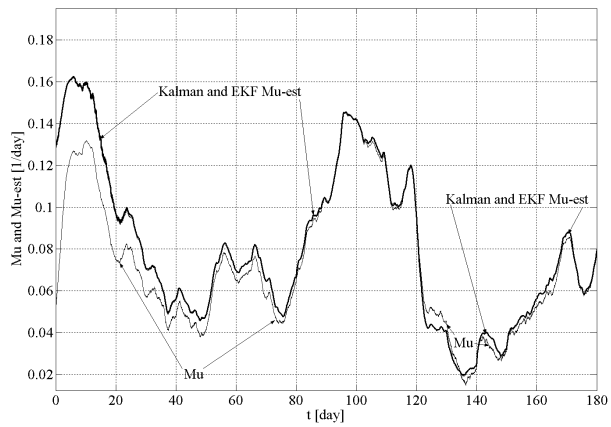
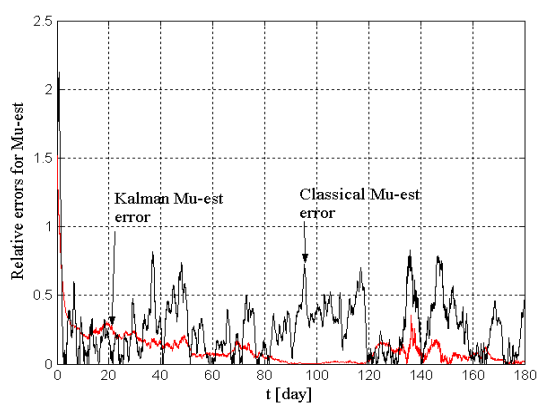


Fig.11. Simulation results with the classical KF and EKF for μ



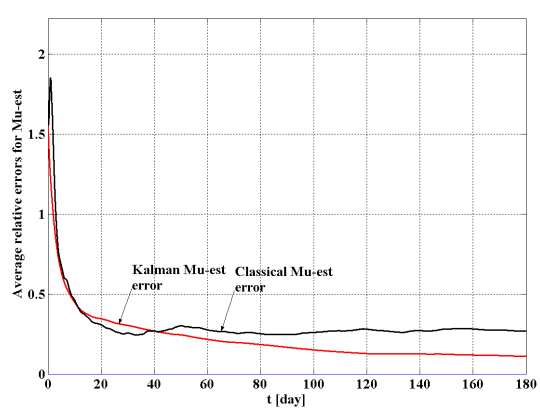


Fig. 12. Relative errors in estimating μ Fig. 13. Average relative errors relevant to Fig. 12 for the KF and classical adjustable soft. sensor

The conducted performance analysis at random perturbations alone (Kalchev et al., 2011) leads to the following conclusions:

- the random perturbations deteriorate the performance of the deterministic software sensors;

- the convergence of the assumed initial estimates of the unmeasurable variables is commensurate for the different software sensors;

- presumably, considerable changes in the state of the nominal (unperturbed) model are harder to be tracked by any of the software sensors. However, smaller changes (as those after simulation day 80) evidence the advantage of the KF over the two equipollent deterministic software sensors.

4.4.2. Performance analysis at random and parameter perturbations

The robustness analysis of considered software sensors should include, besides random perturbations, also parameter perturbations which are due to imprecise parameter identification or to their unpredictable deterministic changes.

The robustness of the same software sensors have been investigated regarding parameters k_1, μ_m and S_{in} at D = 0.06 day^{-1} for the variables μ and X. The perturbations of all the three parameters are applied at days 80 (+20%), 100 (-20%), 120 (-20%) and 140 (+20%).

The conducted simulations at simultaneous random and stepwise parameter perturbations evidence the following conclusions:

- the two deterministic software sensors again are of equal worth but substantially distinct from the KF;

- the KF is more sensitive to a series of parameter perturbations, especially to those of k_1 and S_{in}, in estimating variables μ and X, thus often losing its advantage at random perturbations alone, unless lower values of the parameter perturbations are substantially smaller and possibly rarer ones than those in the simulation studies.

One possibility to overcome the insufficient robustness of the KF to parameter perturbations is the above deterministic software sensor based on EKF. The performance analysis through simulations for it (Kalchev et al., 2009) was made at perturbations of one parameter at a time – k_1 or μ_m, in estimating variables μ and X under the same numerical conditions. The following conclusions were drawn:

- the convergence of the assumed initial estimates to the model variables is much better for the KF;

- the deterministic software sensor based on EKF operates more reliably although not precisely enough at stepwise parameter perturbations.

5. DESIGN OF AN H-INFINITY FILTER AS A SOFTWARE SENSOR FOR THE THREE-STAGE MODEL OF AD

5.1. Theoretical results

The H-infinity filter designed in (Simeonov et al., 2011) presents a peculiar deterministic generalization of the stochastic theory of Kalman filtering, producing estimates of unmeasurable AD biomass and substrate concentrations as time functions which are solutions of the three-stage model (3,4,…8) with specific growth rates μ_1 and μ_2, assumed to be of Monod type, measurable output – biogas flow rate Q, and under random perturbations $w(t)$ and $v(t)$ – components respectively of inlet cattle manure concentration S_{in} and (as measurement noise) of Q.

The H-infinity-optimal estimate $\hat{Y}$ of the state of the linearized three-stage model satisfies the following H-infinity filter equation (Hassibi et al., 1999):

$$\frac{d\hat{Y}}{dt} = A\hat{Y} + e_v^{-1} P C^T (Q - Q_n - C\hat{Y}), \quad \hat{Y}(0) = 0 \tag{28}$$

where A and C are respectively the state and observation matrix of the linearized model; e_v is a scaling factor reflecting the energy of noise $v(t)$; Q_n is the nominal output obtained with the state trajectories in the neighbourhood of which the linearization is made; P is the solution of the following Riccati differential equation:

$$\frac{dP}{dt} = AP + PA^T + BB^T - P(e_v^{-1} C^T C - g^{-2} I)P, \; P(0)$$

where B is the perturbation matrix of the linearized model; $g>0$ is a tuning parameter; I is the relevant identity matrix.

5.2. Simulation studies

The H-infinity filter performance has been evaluated by simulation study comparing its estimates with the respective model variables under pulse changes of dilution rate D and stepwise changes of the constant component of S_{in} (Table 1), under equilibrium model initial condition and

the following constant model parameter values: b=3; Y_p=0.144; μ_{m1}=0.4 day^{-1}; k_{s1}=1.9 g/L; k_1 =6.67; μ_{m2}=0.25 day^{-1}; k_{s2}=0.37 g/L; Y_b=5; k_2= 4.17; Y_g=30.

Both random perturbations *w(t)* and *v(t)* are considered in the simulation study as zero-mean Gaussian white noises with sample times of 1 day and realistically chosen covariance parameter values corresponding to average relative errors of 10% for *w(t)* and of 5% for *v(t)*.

The scaling factor $e_v(t)$ is expressed as $0.0025Q_n^{\,2}(t)$ in terms of the covariance parameter value of *v(t)*.

A selected simulation result concerning the estimation of the variable S_2 of the three-stage model is presented on Fig. 14 demonstrating very good filter's performance.

The following conclusions have been made in the H-infinity filter performance evaluation:

- the estimation of model intermediate substrates S_0, S_1 and S_2 (from noisy measurement only of the biogas flow rate) is of high quality, better than that of model bacterial concentrations X_1 and X_2 due to specific nonlinearities;

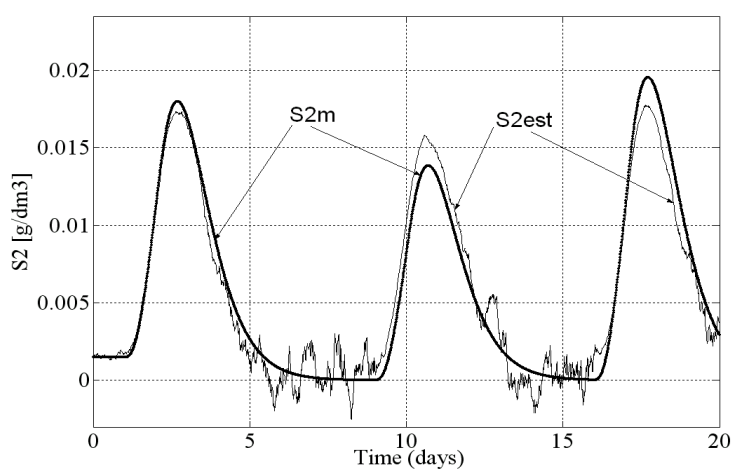


Fig. 14. H-infinity estimation of the variable S_2

- the H-infinity filter is a particularly suitable software sensor in this case due to its advantage over the KF to require no statistical information on random perturbations, which is the case in bioprocess modeling.

6. CONCLUSION

The proposed software sensors for AD unmeasurable variables are model dependent. On the other hand, the one-stage model could also be considered the last stage of all the AD higher-order models used here for software sensor design. The measurement feasibility of Q and D is common in all design cases.

The conducted comparative simulation study of various software sensors on the basis of KF for estimating the unmeasurable variables concentration of methanogenic bacteria (X) and concentration of acetate (S) in a continuous AD process modeled by the one-stage model leads to the conclusion that the classical KF overperforms deterministic software sensors for random perturbations alone, but in case of simultaneous stepwise parameter perturbations it should be upgraded to combine deterministic and stochastic software sensor properties in order to be robust. Such a perspective possibility, although still not elaborated enough, is the deterministic software sensor based on EKF. Another possibility developed in recent years and demonstrated here on the three-stage model, is an H-infinity filter (estimating biomass and substrate concentrations) the convergence of which should be improved for estimating biomass concentrations. Both possibilities require no statistical information on random perturbations, which makes them suitable for AD process monitoring.

Differential algebraic software sensors for estimation of acidogenic and methanogenic bacterial concentrations and specific growth rates have been designed on the basis of the three-stage AD model. They are much simpler than those in (Dochain and Vanrolleghem, 2001) and easily realizable, measuring biogas flow rate and, either methane and carbon dioxide levels in the biogas, or acetate concentration. It is quite evident that only the specific growth rate of methanogenic bacteria μ_2 does not depend on the model parameters adopted for the software sensor design. The performances of the other differential algebraic sensors depend on the precise values of some model parameters.

In order to implement the differential algebraic software sensor for μ_1 and X_1 on the basis of the three-stage model with measurement of S_2, it is necessary to estimate the first derivative of S_2. This is done using regularized numerical differentiation and leads to noise increase in the estimation.

Differential algebraic software sensors based on the AD five-stage model are currently not feasible due to the impossibility to measure hydrogenotrophic and acetoclastic methanogenic bacterial substrate concentrations.

The full experimental validation of these software sensors in strict terms is practically impossible, since it is impossible to measure acidogenic and metanogenic bacterial concentrations. However, the realistic simulations compared with experimental data for the measured biogas, methane and carbon dioxide flow rates show the good performances of the proposed software sensors and present their indirect validation.

The experimental validation of the above presented software sensors is under investigation on a pilot-scale anaerobic CSTR with a computer monitoring system.

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