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Modelling a full scale UASB reactor using a COD global balance approach and state observers

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ABSTRACT

The AM2 model proposed by Bernad et al. [O. Bernad, Z. Hadj-Sadok, D. Dochain, A. Genovesi, J.P. Steyer, Dynamical model development and parameter identification for an anaerobic wastewater treatment process, Biotechnol. Bioeng. 75 (4) (2001) 424–438] was developed as a simple model to simulate wastewater anaerobic digestion. In order to apply this model to a full scale UASB reactor, global COD balance was done. This allows us to determine the stoichiometric coefficients. Using an asymptotic observer biomass content estimation was done without knowledge about the reaction kinetics. Then, a decoupled parameter estimation procedure was followed to determine the evolution of specific growth coefficients. The model and parameters validation was done using experimental data of methane production.

1. Introduction

Since the last decade, dynamical modelling of anaerobic digestion has become an active research area. An important development was the IWA ADM1 [2]. This structured model includes multiple steps describing biochemical and physicochemical processes, involving at least 26 dynamics state variables and many parameters. Although the complexity of anaerobic processes is reflected in the ADM1 model, the direct application for modelling and control purposes is difficult. The identification of model parameters in real conditions is virtually an impossible task. Other simple models were proposed to model anaerobic processes with a reduced set of state variables and parameters [1,3–6]. Although simple models do not represent the complexity of real process, parameter identification and model validation are more straightforward than with ADM1. Generally, these models are implemented based on completely stirred tank reactor (CSTR) conditions. Few authors have considered other hydrodynamic behaviours [7–9].

The AM2 model proposed by Bernard et al. [1] is a two-step (acidogenesis–methanisation) mass-balance model. In the first step, the acidogenic bacteria (X_1) consume the organic substrate (S_1) and produce volatile fatty acids (VFA, S_2) and CO_2 (and more bacteria). Next, methanogenic population (X_2) consumes VFA and produce methane and CO_2 (and more micro-organisms). The biological reactions are

$$k_1S_1 \rightarrow X_1 + k_2S_2 + k_4CO_2 \tag{1}$$

$$k_3S_2 \rightarrow X_2 + k_5CO_2 + k_6CH_4 \tag{2}$$

where S_1 represents the concentration of complex organic substrate (expressed as gCOD/L), S_2 is the concentration of the VFA (expressed as mmolHAc/L), X_1 and X_2 are the concentrations of acidogenic and methanogenic populations (as gVSS/L). The reaction rates are, respectively:

$$r_1 = \mu_1X_1 \tag{3}$$

$$r_2 = \mu_2X_2 \tag{4}$$

where μ_i (in d^{-1}) are the specific growth rates of both micro-organisms types. The other state variable considered is the inorganic carbon concentration (C). Additional model assumptions are: acid–base equilibriums and phase equilibriums, it is considered that inorganic carbon is constituted by CO_2 and bicarbonate (B), and total alkalinity is composed by bicarbonate alkalinity and VFA. In normal pH conditions VFA are completely dissociated; methane is slightly soluble and it is released instantaneously, and CO_2 follows Henry's law. CSTR behaviour is assumed for the liquid phase. In order to incorporate the effect of solids retention in the reactor, the authors introduce the α parameter, which represents the solid fraction that leaves the reactor. Then, equations of the dynamical model are

$$\frac{dX_1}{dt} = [\mu_1(\xi) - \alpha D]X_1 \tag{5}$$

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$$\frac{dX_2}{dt} = [\mu_2(\xi) - \alpha D]X_2 \tag{6}$$

$$\frac{dS_1}{dt} = D(S_{1\text{in}} - S_1) - k_1\mu_1X_1 \tag{7}$$

$$\frac{dS_2}{dt} = D(S_{2\text{in}} - S_2) + k_2\mu_1X_1 - k_3\mu_2X_2 \tag{8}$$

$$\frac{dC}{dt} = D(C_{\text{in}} - C) - q_C + k_4\mu_1X_1 + k_5\mu_2X_2 \tag{9}$$

where D is the dilution rate (in d^{-1}), q_C is the CO_2 flux (in mmol/(L d)) and the in subindex show inlet conditions. The model can be rewritten in a more compact matrix form as

$$\frac{d\xi}{dt} = Kr(\xi) - Dx - Q + F \tag{10}$$

where

$$\xi = \begin{bmatrix} X_1 \\ X_2 \\ S_1 \\ S_2 \\ C \end{bmatrix}, \qquad r(\xi) = \begin{bmatrix} \mu_1(\xi)X_1 \\ \mu_2(\xi)X_2 \end{bmatrix}, \qquad K = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -k_1 & 0 \\ k_2 & -k_3 \\ k_4 & k_5 \end{bmatrix},$$

$$F = \begin{bmatrix} 0 \\ 0 \\ DS_{1\text{in}} \\ DS_{2\text{in}} \\ DC_{\text{in}} \end{bmatrix}, \qquad Q = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ q_C(\xi) \end{bmatrix}, \qquad D = \begin{bmatrix} \alpha D & 0 & 0 & 0 & 0 \\ 0 & \alpha D & 0 & 0 & 0 \\ 0 & 0 & D & 0 & 0 \\ 0 & 0 & 0 & D & 0 \\ 0 & 0 & 0 & 0 & D \end{bmatrix}$$

An additional equation of the model give the methane flux q_M:

$$q_M = k_6\mu_2X_2 \tag{11}$$

The parameter identification procedure followed by Bernard et al. [1] is based on steady state variables values determination. Then, they correlated them by equations coming from the model assumptions. This is a valid approach for a highly controlled reactor like a pilot or bench scale reactor, but is unrealistic for a full-scale reactor. In this case, it is difficult to reach true steady states because of inlet flow and concentration disturbances. Another approach is proposed in this paper based on global COD balances from S_1 and S_2, applied to a 250-m^3 reactor treating malting plant effluent [10]. After k_1, k_2, k_3 and k_6 determination, an asymptotic observer [11] is used to estimate biomass concentration without knowledge about the reaction kinetics. Observers provide software measurements of unmeasured variables or unknown parameters on the basis of the knowledge of the process dynamics. Asymptotic observers are based in a linear transformation of state variables that allow write the material balance in a form independent of the reaction kinetic. Using a decoupled parameter estimation [12], the evolution of specific growth coefficients is determined simultaneously. Finally, stoichiometric coefficients related to CO_2 production were determined.

2. Materials and methods

A full scale UASB reactor of 250 m^3 [10] for treatment of malting plant effluent was monitored during 180 days (Fig. 1). The wastewater to be treated comes from the steeping process of a malting plant. Its average flow rate is of 350 m^3/d. The average concentration of the stream is around 2400 mgCOD/L. Working temperature is clearly determined by the industrial process temperature and was around 20 °C. For monitoring purposes COD, VFA and alkalinity were measured at the inlet and outlet of the reactor. COD was determined by the reflux method [13] and VFA and alkalinity by a simplified method proposed by DiLallo and Albertson [14]. The pH, temperature and flow rates (liquid and gas) were registered online using the industrial plant SCADA system. The biogas production was established through out time and gas chromatography was performed to determine its composition. Samples of the sludge bed were periodically collected from different depths and solid content in the reactor were determined. In the considered period the volumetric organic load was around 4 kgCOD/(m^3 d) and the specific organic load was between 0.2 and 0.4 kgCOD/(kgVSS d). COD removal efficiency was 80%.

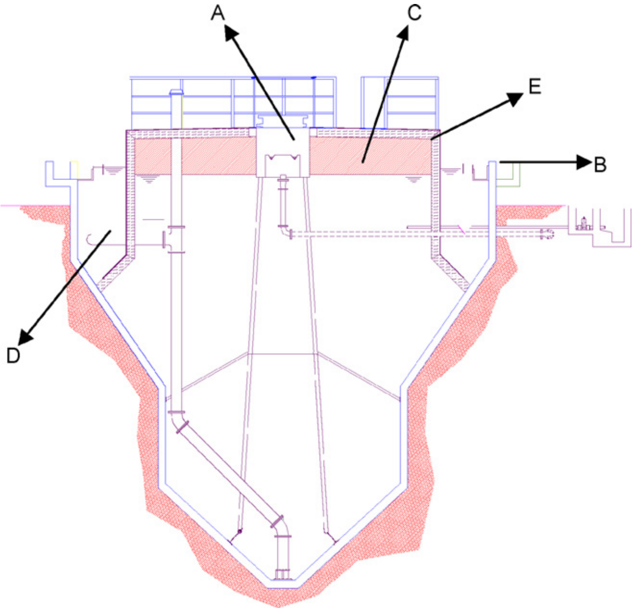

Fig. 1. Reactor scheme: (A) inlet chamber; (B) outlet; (C) gas collection chamber; (D) sludge purge; (E) steel structure.

Taking into account the whole period studied, mass balances are performed to determine the stoichiometrics coefficients. The organic matter S_1 removed in this period was calculated from the difference between the accumulated organic matter at the inlet and at the outlet. In a similar way, the volatile fatty acids (S_2) difference between the exit and the inlet is calculated. In addition, accumulated methane production and solid growth in the reactor are registered.

Asymptotic observers can be used if stoichiometric coefficients are known. Using these observers there is no need to know the kinetic expressions [11]. In this way, S_1, S_2, X_1 and X_2 can be estimated through out time and then compared with the measured data. From the general equation:

$$\frac{d\xi}{dt} = Kr(\xi) - D\xi - Q + F \tag{12}$$

a subset of variables $x = [S_1\ S_2\ X_1\ X_2]$ are considered. Then, the following state partition is defined: $x_1 = [S_1\ S_2]$, the measured variables and $x_2 = [X_1\ X_2]$, the variables to estimate. The others matrix are partitioned in a similar way.

$$K_1 = \begin{bmatrix} -k_1 & 0 \\ k_2 & -k_3 \end{bmatrix}, \qquad K_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad F_1 = \begin{bmatrix} DS_{1\text{in}} \\ DS_{2\text{in}} \end{bmatrix},$$

$$F_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad Q = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad D_1 = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}, \qquad D_2 = \alpha \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix}$$

The former equations can be rewritten as follows:

$$\dot{x}_1 = K_1r(x) - Dx_1 + F_1 \tag{13}$$

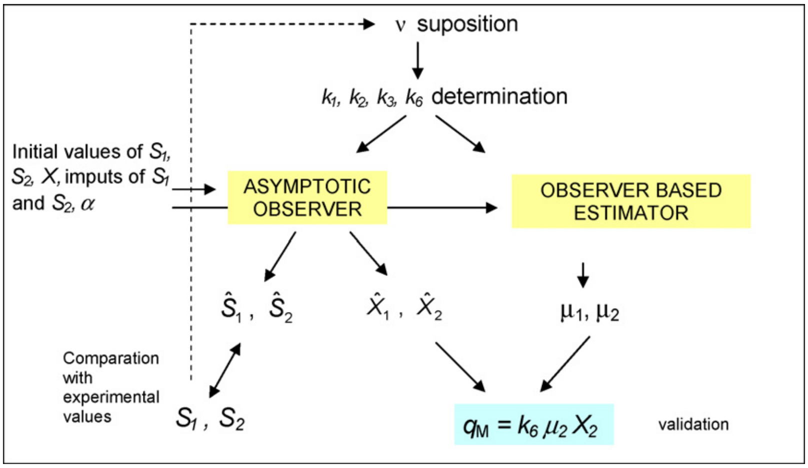

Fig. 2. Algorithm for stoichiometric and kinetic parameters estimation.

$$\dot{x}_2 = K_2 r(x) - \alpha D x_1 \tag{14}$$

As K_1 is full rank the following matrix can be defined:

$$C = K_2 K_1^{-1} = -\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\dfrac{1}{k_1} & 0 \\ \dfrac{k_2}{k_1 k_3} & -\dfrac{1}{k_3} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{k_1} & 0 \\ -\dfrac{k_2}{k_1 k_3} & \dfrac{1}{k_3} \end{bmatrix} \tag{15}$$

also the following state transformation can be defined

$$h = x_2 - K_2 K_1^{-1} x_1 = x_2 + C x_1 \tag{16}$$

and its derivative

$$\dot{h} = \dot{x}_2 + C\dot{x}_1 = -\alpha D x_2 + C(-D x_1 + F_1) \tag{17}$$

It can be observed that h does not depend on the reaction kinetics. In this case:

$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} X_1 + \dfrac{S_1}{k_1} \\ X_2 - \dfrac{k_2}{k_1 k_3} S_1 + \dfrac{S_2}{k_3} \end{bmatrix},$$

$$\begin{bmatrix} \dot{h}_1 \\ \dot{h}_2 \end{bmatrix} = \begin{bmatrix} D\left(\dfrac{S_{1\text{in}} - S_1}{k_1} - \alpha X_1\right) \\ D\left(\dfrac{k_2}{k_1 k_3}(S_{1\text{in}} - S_1) + \dfrac{S_{2\text{in}} - S_2}{k_3} - \alpha X_2\right) \end{bmatrix} \tag{18}$$

Then, knowing inlet and outlet values of S_1 and S_2, X_1 and X_2 can be estimated:

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} h_1 - \dfrac{S_1}{k_1} \\ h_2 + \dfrac{k_2}{k_1 k_3} S_1 - \dfrac{S_2}{k_3} \end{bmatrix} \tag{19}$$

Simultaneously, an observer-based estimator is proposed for kinetic parameters estimation [11,12]. Taking the transformation $z = K_1^{-1} x$ the estimator is

$$\frac{\mathrm{d}\hat{z}_1}{\mathrm{d}t} = \hat{\mu}_1 X_1 - D z_1 - D\frac{S_{1\text{ in}}}{k_1} + \omega_1(z_1 - \hat{z}_1) \tag{20}$$

$$\frac{\mathrm{d}\hat{\mu}_1}{\mathrm{d}t} = \gamma_1(z_1 - \hat{z}_1) \tag{21}$$

$$\frac{\mathrm{d}\hat{z}_2}{\mathrm{d}t} = \hat{\mu}_2 X_2 - D z_2 - D\left(\frac{k_2}{k_1 k_3} S_{1\text{in}} + \frac{S_{2\text{in}}}{k_3}\right) + \omega_2(z_2 - \hat{z}_2) \tag{22}$$

$$\frac{\mathrm{d}\hat{\mu}_2}{\mathrm{d}t} = \gamma_2(z_2 - \hat{z}_2) \tag{23}$$

where the “hat” variables are the estimated ones and ω_i and γ_i are the gains of the observer. Following Perrier et al. [12] suggestion $\gamma_i = \omega_i^2/4$ can be taken. Then, only two parameters can be adjusted.

Fig. 2 shows the algorithm for parameters estimation. A supposed value of ν (acidogenic fraction of biomass) gives k_i stoichiometrics coefficients. Using the asymptotic observer (Eq. (18)) and knowing initial values of state variables and input variables throughout time we can solve the differential equations. Estimated values of state variables S_1 and S_2 are compared with experimental values and optimisation of ν value can be achieved. Simultaneously the integration of Eqs. (20)–(23) gives μ_i kinetic parameters evolution. Finally, knowing μ_2 and X_2 we can estimate methane flux using Eq. (11) and perform the model validation with experimental biogas values.

In order to determine the stoichiometric coefficients k_4 and k_5 Eq. (9) was integrated. The experimental values of q_C and C_{in} and estimated values of μ_i and X_i, were used. Calculated C was compared with experimental values using a least squares criterion.

The calculating algorithms and the optimisation runs were implemented using MATLAB®.

3. Results and discussion

Integration of substrates and products flows in the studied period gives the following results, expressed as mass per litre of reactor:

- S_1 removed: 360 gCOD
- ΔS_2 (inlet – outlet): 789 mmol (50 gCOD)
- Methane produced: 5816 mmol (372 gCOD)
- $\Delta X = 21.5$ gVSS

where $X = X_1 + X_2$. We define ν as the acidogenic fraction of total biomass. Then, $\Delta X_1 = \nu\,\Delta X$, $\Delta X_2 = (1-\nu)\Delta X$. Performing COD balances for the studied period:

- Reaction 1: (S_1 removed) = (S_2 produced) + (X_1 produced)
- Reaction 2: (S_2 consumed) = (Methane produced) + (X_2 produced)

or, expressed as gCOD per litre of reactor

- Reaction 1: $360 = (360 - a) + a$
- Reaction 2: $(372 + b) = 372 + b$

where a is the amount of S_1 that is converted to X_1, b is the amount of S_2 that is converted to X_2 expressed as gCOD/L. Performing a mass

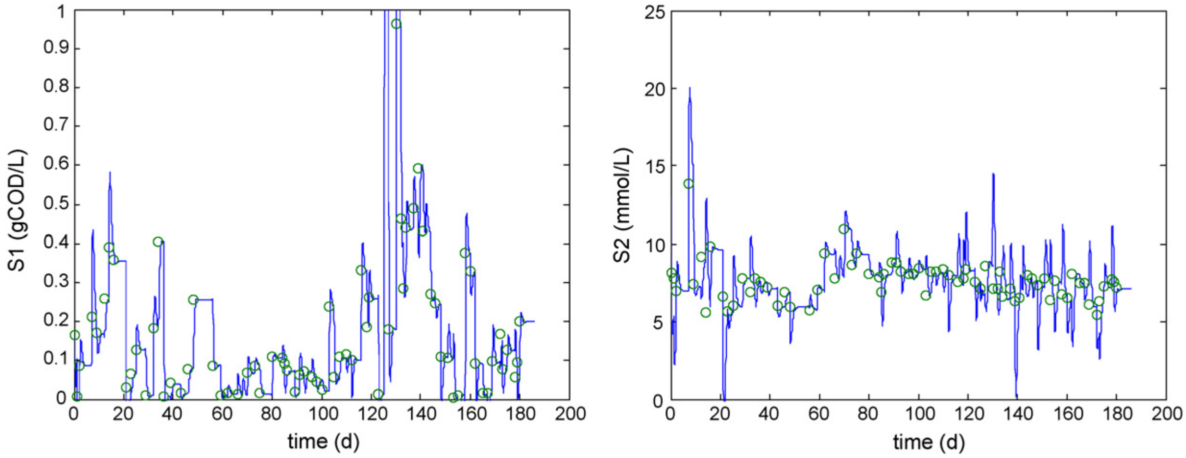

Fig. 3. Simulated and experimental substrate and VFA concentration in the reactor throughout time.

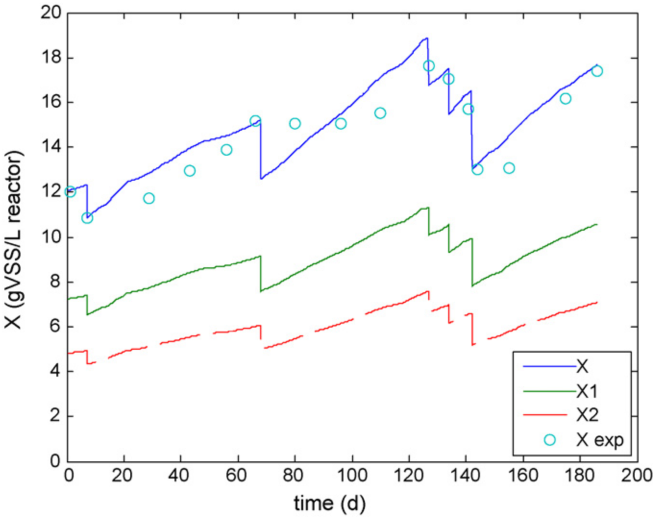

Fig. 4. Simulated and experimental VSS content in the reactor throughout time.

balance for S_2:

$(S_2 \text{ produced in reaction 1}) + \Delta S_2 = (S_2 \text{ consumed in reaction 2})$

or

$(360 - a) + 50 = 372 + b \Rightarrow a + b = 38\,\text{gCOD}$

It must be noticed that the experimental factor of biomass conversion to COD is 38 gCOD/21.5 gVSS = 1.76 gCOD/gVSS, considerable higher than common value of 1.42 gCOD/gVSS, and in accordance with other authors [15]. It is assumed that a and b are at the same proportion than X_1 and X_2. Then, $a = 38\nu$, $b = 38(1 - \nu)$ expressed as gCOD per litre of reactor. The stoichiometric coefficients are

$$
\begin{aligned}
k_1 &= (S_1 \text{ removed})/\Delta X_1 = 360/(\nu \cdot 21.5)\text{gCOD/gVSS}\\
k_2 &= (S_2 \text{ produced in reaction 1})/\Delta X_1\\
&= (360 - a)/(\nu \cdot 21.5)\text{gCOD/gVSS}\\
k_3 &= (S_2 \text{ removed in reaction 2})/\Delta X_2\\
&= (372 + b)/((1 - \nu)21.5)\text{gCOD/gVSS}\\
k_6 &= (\text{Methane produced})/\Delta X_2\\
&= 5816/((1 - \nu)21.5)\text{mmol CH}_4\text{/gVSS}
\end{aligned}
$$

Then, the stoichiometric coefficients k_1, k_2, k_3 and k_6, and biomass concentrations X_1 and X_2 are exclusively functions of ν. In a stable situation, the ν value can be considered constant.

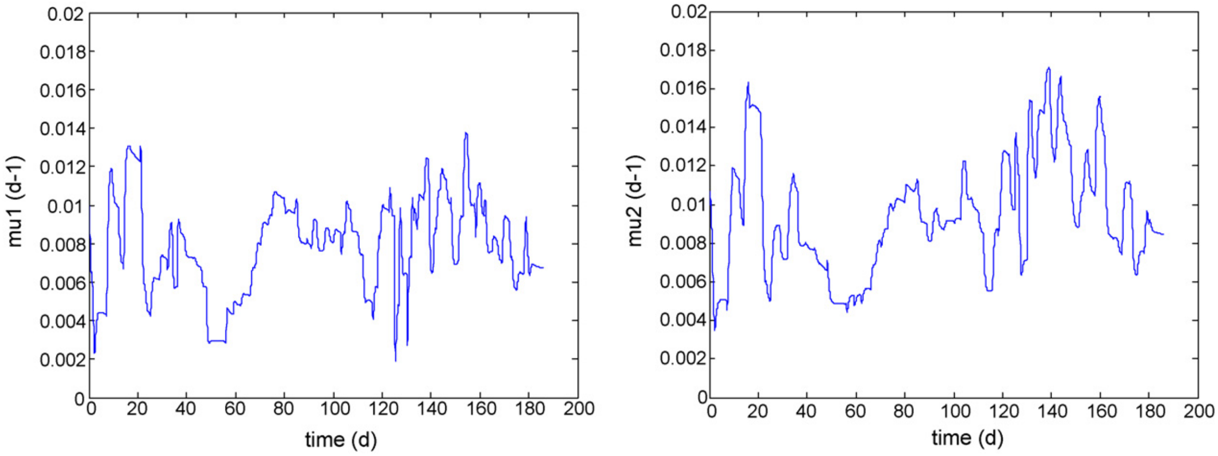

Fig. 5. Kinetic specific rates evolution throughout time.

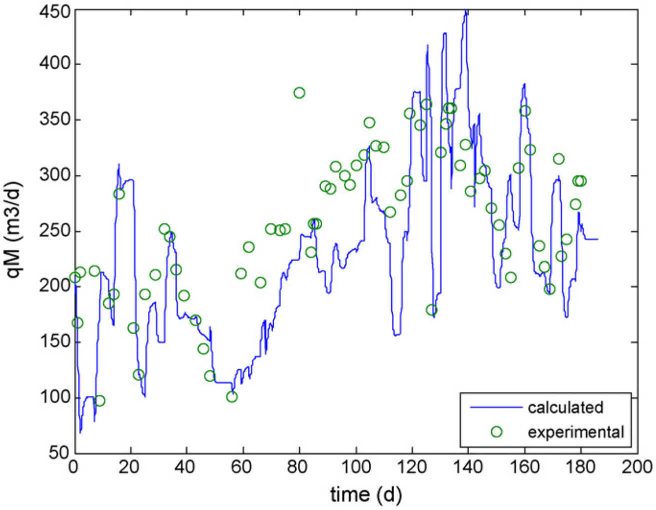

Fig. 6. Simulated and experimental methane production data throughout time.

Knowing the initial values of the state values, the stoichiometric coefficients and the α parameter, it is possible to solve the differential equations system. As the stoichiometric coefficients are exclusively depending on ν parameter, system optimisation can be easily done adjusting with experimental S_1 and S_2 values. In this case, $S_{1o} = 0.165$ gCOD/L, $S_{2o} = 8.13$ mmol/L, $X_o = 12.02$ gVSS/L (referred to the reactor volume). Besides, the inlet data (S_{1in} and S_{2in}) are known.

Taking into account an experimental average of 0.25 mL/L of Sedimented solids in the exit, with a density of 50 gVSS/L, and an average content of solids of 3580 kgVSS in the reactor, a value of $\alpha = 0.0012$ was estimated. This small α value shows that retention of solids in the reactor is very efficient. Then, ΔX value is a reasonable measure of the biomass growth.

Initial values for growth coefficients of $\mu_{1o} = \mu_{2o} = 0.01\ \mathrm{d}^{-1}$ were taken and values of $\omega_1 = \omega_2 = 4.5$ were chosen for the observer gain. Using a least squares criterion a value of $\nu = 0.6$ was found and model results are in agreement with experimental values of S_1 and S_2 (Fig. 3). Therefore, values of $k_1 = 27.9$ gCOD/gVSS, $k_2 = 408$ mmol/gVSS, $k_3 = 703$ mmol/gVSS and $k_6 = 676$ mmol/gVSS were obtained. In Fig. 4 simulated and experimental data of VSS in the reactor are shown. Sludge purges performed in the reactor were taking into account.

Fig. 5 shows specific rates evolution throughout time. As the correlation between the kinetic values and the substrate concentration is not good, it is not possible to adjust a Monod or a Haldane kinetic. As a consequence, in this work it is necessary to use the specific rates instead of the kinetic expressions.

In order to validate the parameters determined and the model proposed, methane production can be calculated using Eq. (11). A good correlation between experimental and simulated data is observed in Fig. 6.

Finally, Eq. (9) was integrated to determine the stoichiometric coefficients k_4 and k_5. Using a least squares criterion to minimize the difference, optimal values of the coefficients were obtained: $k_4 = 431$ mmol/gVSS and $k_5 = 37$ mmol/gVSS.

4. Conclusions

An alternative approach to simulate full-scale reactor behaviour using the AM2 model was presented. Based on global COD balances performed in the reactor during a period, stoichiometric coefficients were determined. As an asymptotic observer was used, there was no need to know the kinetic expressions in order to estimate the acidogenic and methanogenic biomass content in the reactor. The decoupled parameter estimation using an observer-based estimator allows to determine kinetic values through out time. Finally, well fitting of experimental and calculated methane production allows to validate the model proposed and parameter estimation.

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