Modelling and Identification of a Distributed-Parameter System for an Anaerobic Wastewater Treatment Process

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Abstract – The objective of this study is to develop a distributed-parameter model for an anaerobic wastewater treatment process with a view of monitoring and control of the process. In particular the model could possibly be used as part of a diagnosis tool for process failure such as clogging. It will be used in a sensor location study. And it could also be considered in the design of advanced control strategies. The methodology follows three steps: 1) converting a validated uniformed-parameter model into a distributed-parameter model, 2) calibrating it using steady-state data, and 3) validating under transient conditions. Simulation results reveal that the distributed-parameter model allowed describing experimental data with at least the same performance as with the uniformed-parameter model. The dynamics of the biomass within the reactor can be described by the distributed-parameter model, and the study of the biomass profile documented experimental clogging observations.

I. INTRODUCTION

Anaerobic digestion is a widely-used wastewater treatment process because of its ability to degrade concentrated and difficult substrates [MAT, 00]. However, anaerobic digestion is also known to become easily unstable in presence of variations of operating conditions [FRI, 84]. Moreover, when operated over long periods of time, clogging of the bioreactor may occur. In order to cope with these problems, control strategies can be implemented that maintain the process under optimal conditions. This implies the development of a mathematical model that is, on one hand, reliable and robust, and on the other hand, easy to calibrate (in order to be used for control purposes). The mathematical representation of anaerobic digestion process dynamics has been largely investigated in the literature and many phenomenological models have been developed that consider several bacterial populations and several substrates [KIE, 97]. Such models typically contain too many parameters leading to identification problems. In [BER, 01], a reduced-order model, based on two microbial populations and two substrates, has been developed and proved to be reliable and robust, in particular during abnormal operating conditions. One drawback of this model is that it assumes the process to behave like a continuously stirred tank reactor (CSTR). In practice, in fixed or fluidized bed reactors, liquid phase concentrations may be assumed to be uniform within the reactor under specific hydrodynamic conditions. Yet fixed biomass can be spatially distributed and a biomass gradient can take place. This may lead in some instances to clogging problems [HAR, 02]. In such instances, the development of a distributed-parameter model may be useful 1) to better describe what happens in the reactor, 2) to study the influence of hydrodynamic conditions, 3) to predict clogging, and 4) to implement robust control strategies.

This paper is organized as follows. The lumped-parameter model equations will first be recalled and the deduced distributed-parameter model will be introduced in Section 2. Then, the experiments that have led to the calibration and validation data will be described in Section 3. The calibration and the validation of the distributed–parameter model, as well as the comparison of both models, will be presented in Section 4. Finally, some conclusions and perspectives will be given in Section 5.

II. MATHEMATICAL DEVELOPMENTS

The full reduced-order model of anaerobic digestion developed in [BER, 01] is given by the following equations:

$$\frac{dX_1}{dt} = (\mu_1 - \alpha \cdot D) \cdot X_1 \qquad (1)$$

$$\frac{dX_2}{dt} = (\mu_2 - \alpha \cdot D) \cdot X_2 \qquad (2)$$

$$\frac{dZ}{dt} = D \cdot \left(Z_{in} - Z\right) \tag{3}$$

$$\frac{dS_1}{dt} = D \cdot \left(S_{1in} - S_1\right) - k_1 \cdot \mu_1 \cdot X_1 \tag{4}$$

$$\frac{dS_2}{dt} = D \cdot \left(S_{2in} - S_2\right) + k_2 \cdot \mu_1 \cdot X_1 - k_3 \cdot \mu_2 \cdot X_2 \tag{5}$$

$$\frac{dC}{dt} = D \cdot \left(C_{in} - C\right) - q_C + k_4 \cdot \mu_1 \cdot X_1 + k_5 \cdot \mu_2 \cdot X_2 \tag{6}$$

with

$$\mu_1 = \mu_{1\max} \cdot \frac{S_1}{K_{S1} + S_1} \tag{7}$$

$$\mu_2 = \mu_{2s} \cdot \frac{S_2}{K_{S2} + S_2 + \frac{S_2^2}{K_{I2}}} \tag{8}$$

$$q_C = k_L a \cdot \left(C + S_2 - Z - K_H \cdot P_C\right) \tag{9}$$

where

$$P_C = \frac{\phi - \sqrt{\phi^2 - 4 \cdot K_H \cdot P_T \cdot \left(C + S_2 - Z\right)}}{2 \cdot K_H} \tag{10}$$

with

$$\phi = C + S_2 - Z + K_H \cdot P_T + \frac{k_6}{k_L a} \cdot \mu_2 \cdot X_2 \tag{11}$$

$$q_M = k_6 \cdot \mu_2 \cdot X_2 \tag{12}$$

$$pH = -\log_{10}\left(K_b \cdot \frac{C - Z + S_2}{Z - S_2}\right) \tag{13}$$

where S_1 represents the organic substrate (characterized by its chemical oxygen demand, COD), S_2 denotes the volatile fatty acids (VFA); X_1 and X_2 are the acidogenic and methanogenic bacteria, respectively; μ_1 and μ_2 represent the specific growth rates of acidogenesis and methanization, respectively; Z and C are the total alkalinity and the total inorganic carbon, respectively; k_1, k_2, k_3, k_4, k_5 and k_6 are yield coefficients; μ_{1max}, μ_{2s}, K_{S1}, K_{S2}, and K_{I2} are biokinetic parameters; k_La is the liquid-gas transfer coefficient; K_H is the Henry's constant; Pc and P_T are the carbon dioxide and the total pressure, respectively; q_C and q_M are the carbon dioxide and methane flow rates, respectively; K_b is the an affinity constant; D is the dilution rate; and α is the fraction of bacteria in the liquid phase.

The distributed-parameter model is obtained by introducing the hydrodynamic terms for a tubular reactor with axial dispersion, as follows:

$$\frac{\partial X_1}{\partial t} = \left(\mu_1 - \alpha \cdot D\right) \cdot X_1 \tag{14}$$

$$\frac{\partial X_2}{\partial t} = \left(\mu_2 - \alpha \cdot D\right) \cdot X_2 \tag{15}$$

$$\frac{\partial Z}{\partial t} = -u_l \cdot \frac{\partial Z}{\partial z} + E_z \cdot \frac{\partial^2 Z}{\partial z^2} \tag{16}$$

$$\frac{\partial S_1}{\partial t} = -u_l \cdot \frac{\partial S_1}{\partial z} + E_z \cdot \frac{\partial^2 S_1}{\partial z^2} - k_1 \cdot \mu_1 \cdot X_1 \tag{17}$$

$$\frac{\partial S_2}{\partial t} = -u_l \cdot \frac{\partial S_2}{\partial z} + E_z \cdot \frac{\partial^2 S_2}{\partial z^2} + k_2 \cdot \mu_1 \cdot X_1 - k_3 \cdot \mu_2 \cdot X_2 \tag{18}$$

$$\frac{\partial C}{\partial t} = -u_l \cdot \frac{\partial C}{\partial z} + E_z \cdot \frac{\partial^2 C}{\partial z^2} - q_C + k_4 \cdot \mu_1 \cdot X_1 + k_5 \cdot \mu_2 \cdot X_2 \tag{19}$$

with

$$\mu_1 = \mu_{1\max} \cdot \frac{S_1}{K'_{S1} \cdot X_1 + S_1} \tag{20}$$

$$\mu_2 = \mu_{2s} \cdot \frac{S_2}{K'_{S2} \cdot X_2 + S_2 + \frac{S_2^2}{K_{I2}}} \tag{21}$$

$$q_C(z + dz) = q_C(z) + k_L a \cdot (A \cdot dz) \cdot \left(C(z) + S_2(z) - Z(z) - K_H \cdot P_C(z)\right) \tag{22}$$

where

$$P_C = \frac{\phi(z) - \sqrt{\phi(z)^2 - 4 \cdot K_H \cdot P_T(z) \cdot \left(C(z) + S_2(z) - Z(z) + \frac{q_C(z - dz)}{k_L a \cdot dV}\right)}}{2 \cdot K_H} \tag{23}$$

with

$$P_T(z) = P_T + \rho \cdot g \cdot (H - z) \tag{24}$$

$$\phi(z) = C(z) + S_2(z) - Z(z) + K_H \cdot P_T(z) + \frac{q_M(z) + q_C(z - dz)}{k_L a \cdot dV} \tag{25}$$

$$q_M(z + dz) = q_M(z) + k_6 \cdot \mu_2 \cdot X_2(z) \cdot A \cdot dz \tag{26}$$

$$pH(z) = -\log_{10}\left(K_b \cdot \frac{C(z) - Z(z) + S_2(z)}{Z(z) - S_2(z)}\right) \tag{27}$$

where A is the cross section area; u_L is the liquid velocity and E_z is the axial dispersion coefficient.

Remark : Note that a Contois-based relationship (and not the more classical Monod or Haldane type structures) has been introduced into the microbial growth kinetics. This choice is motivated by two arguments.

1) it is important to note that the choice of kinetic models for the specific growth rates that only depend on the limiting substrate concentrations (i.e. here S_1 for the acidogenesis, and S_2 for the methanization) leads to model for which the only admissible steady-state profile is with no biomass (i.e. here $X_1 = X_2 = 0$) (this is straightforward when examining equations (1) and (2)). The introduction of the term that depends on the biomass concentration in the specific growth rate model allows to circumvent this problem and generate other (and of "physical" and practical interest) steady-states, i.e. non-zero biomass concentrations. It is also worth noting that multiplicity of the steady-states can be emphasized with the modified Haldane model, this situation corresponding to the multiplicity of the steady-states in the finite-dimensional case (CSTR).
2) The second argument for introducing the Contois-based formulation of the specific growth rates μ_1 and μ_2 is that this structure allows to emphasize the existence of concentration gradients in steady-states with higher concentrations, of biomass in particular, at the bottom of the reactor with decreasing value at increasing reactor height, or in other words, heavy particles are located at the bottom while the lighter particles are at the top : this is typically the situation experimentally observed.

III. Materials and Methods

The pilot reactor is an anaerobic upflow fixed-bed reactor of 3.5m height and 0.6m diameter. The effective volume of the medium is 0.948 m^3 and the support surface equals 135 m^2 (Cloisonyl: 180 m^2/m^3). The bioreactor is operated with a recycle rate of 50 L/h.

The experimental protocol has been determined in order to cover a wide range of organic loading rates and to obtain situations close to the destabilization of the fermenter. Profiles of the influent parameters are presented in Fig. 1.

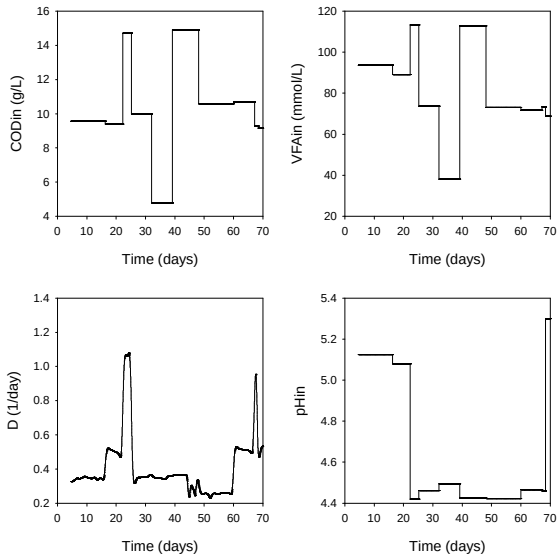

Fig. 1. Profiles of the influent parameters

Details on the reactor, measurements and protocols are available in [BER, 01].

IV. Simulation Results

A. The uniformed-parameter model

Simulation results for the uniformed-parameter model, reported in [BER, 01], are presented in Fig. 2, Fig. 3, and Fig. 4.

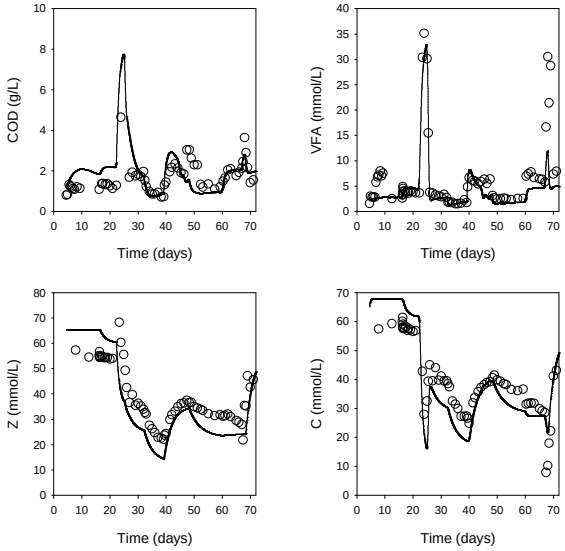

Fig. 2 Measured (○) and simulated (——) data for COD, VFA, alkalinity and total inorganic carbon (uniformed-parameter model)

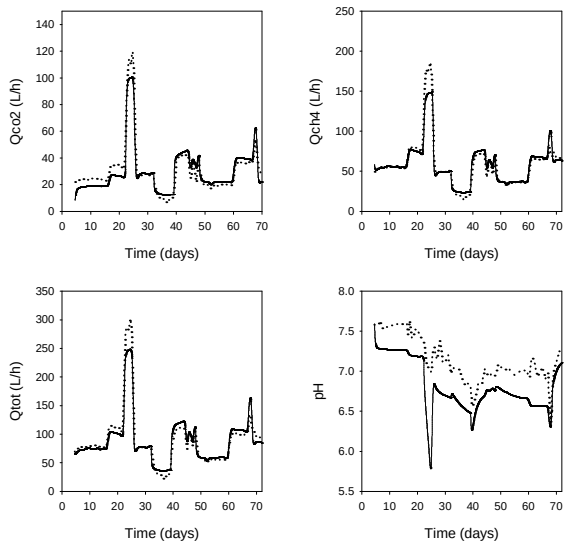

Fig. 3 Measured (.) and simulated (——) data for gaseous flow rates and pH (uniformed-parameter model)

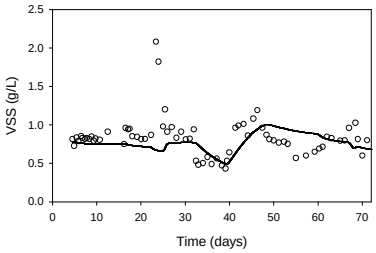

Fig. 4 Measured (○) and simulated (——) data for VSS (uniformed-parameter model).

B. The distributed-parameter model

The hydrodynamic parameters were identified using the data on total alkalinity since it is not consumed within the reactor [BER, 01]. Because the dilution rate is very high, the model is not sensitive with respect to the hydrodynamic parameters so that accurate parameter identification cannot be conducted. Good results were obtained by setting Ez equal to 1. The mean value of the Peclet number is 20, which corresponds to a highly dispersed tubular reactor.

Since a Contois-based kinetics model was introduced in the writing of the microbial growth rates, some biokinetic parameters had to be re-identified. Using the experimental data of VSS, half saturation constants were determined as follows:

$$K'_{S1} = \frac{K_{S1}}{\overline{X}_1} \text{ and } K'_{S2} = \frac{K_{S2}}{\overline{X}_2} \qquad (28)$$

where $\overline{X}_1$ and $\overline{X}_2$ denotes the mean values of the corresponding biomass.

This change had some consequences on the curves that compare experimental data with the simulated model so that k_2, k_3, k_5 and k_6 had to be re-identified using data of steady-states. Values of parameters for both models are summarized in Table 1.

Table 1. Values of parameters for the two models

Parameter	Value - uniformed -	Value - distributed -
μ_{1max} (1/d)	1.2	1.2
K_{S1} (g/L) or K'_{S1} (g S_1/g VSS)	7.1	50.5
μ_{2s}	0.74	0.74
K_{S2} (g/L) or K'_{S2} (g S_2/g VSS)	9.28	16.6
K_{I2} (mmol/L)	256	256
α	0.5	0.5
k_La (1/d)	19.8	19.8
K_H (mol/(L.atm))	16	16
k_1 (g/g)	42.14	42.14
k_2 (mmol/g)	116.5	250
k_3 (mmol/g)	268	134
k_4 (mmol/g)	50.6	50.6
k_5 (mmol/g)	343.6	171.3
k_6 (mmol/g)	453.0	188.75

Simulation results for the distributed-parameter model are presented in Fig. 5, Fig. 6, Fig. 7 and Fig. 8. Space derivatives were approximated using the finite difference method and ten nodes were considered. No significant improvement was obtained when increasing the number of nodes.

Qualitatively, the distributed-parameter model is able to describe experimental data as well as the lumped-parameter model. Moreover, the profile of the biomass concentrations within the reactor can be described by the distributed-parameter model.

Simulation curves of the biomass profile within the reactor tend to show that a gradient concentration takes place (see Fig. 8), and that clogging is more likely to occur at the input of the reactor (z close to zero). This is confirmed by experimental clogging observations [HAR, 02].

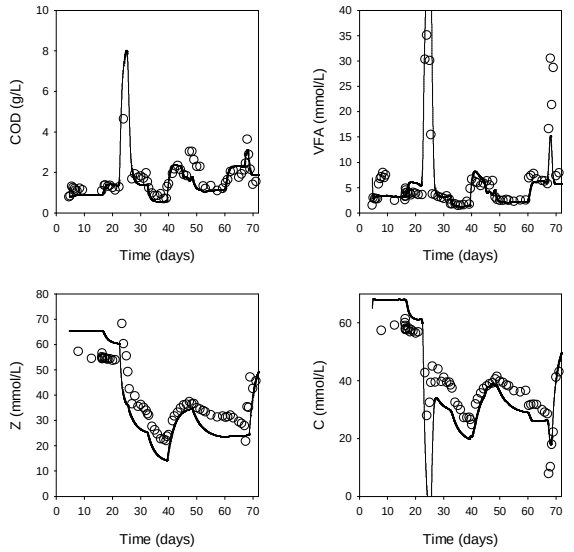

Fig. 5 Measured (○) and simulated (——) data for COD, VFA, alkalinity and total inorganic carbon (distributed-parameter model)

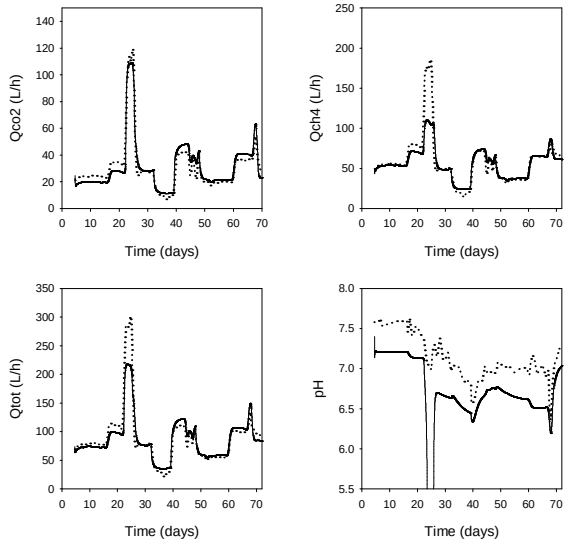

Fig. 6 Measured (.) and simulated (——) data for gaseous flow rates and pH (distributed-parameter model)

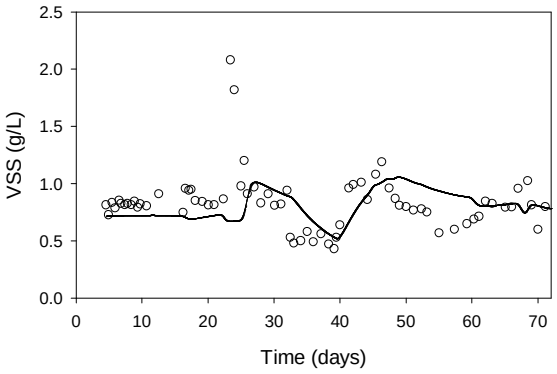

Fig. 7 Measured (○) and simulated (——) data for VSS (distributed-parameter model)

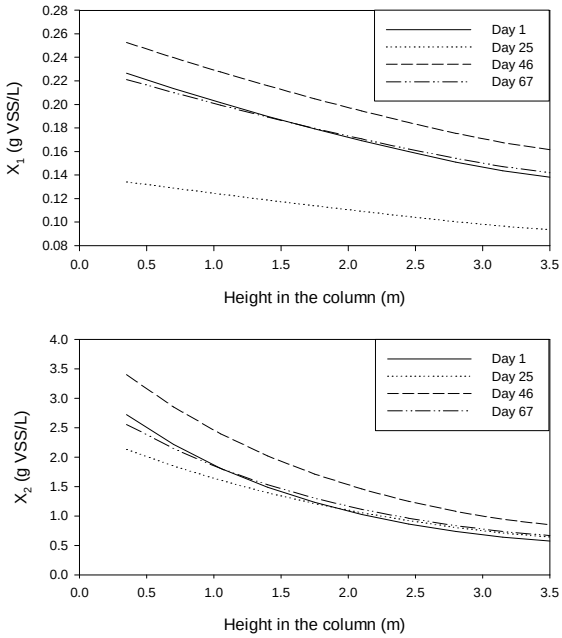

Fig 8. Simulated biomass profiles within the reactor.

In order to compare the performance of both models, the following dimensionless quadratic criterion has been considered:

$$\sigma_y = \frac{1}{t_f}\int_0^{t_f}\left(\frac{\hat{y}(\tau)-y(\tau)}{y(\tau)}\right)^2 d\tau \qquad (29)$$

where $\hat{y}(\tau)$ and $y(\tau)$ are the predicted and actual values of the variable y at time τ, respectively.

The errors for each state variable and for both models are calculated by using the above criterion. The results are presented in Table 2.

Table 2. Simulation errors

Sate variable	Error (%) - uniformed -	Error (%) - distributed -
COD	34.02	16.29
VFA	13.71	59.32
Z	4.58	4.75
C	6.64	9.62
Q_{CO2}	6.45	5.07
Q_{CH4}	2.91	3.90
Q_{tot}	3.53	3.82
pH	0.25	2.79
VSS	9.49	9.07

Simulation errors are similar for all sate variables except for COD and VFA. The error on the COD simulation curve was drastically reduced (from 34% to 16%) due to a better description of the beginning of the experiment and of the destabilization phase occurring at day 24. Surprisingly, even if the distributed-parameter model seems to describe VFA as well as the uniformed-parameter model for most data, the simulation error on VFA is increased (from 14% to 59%). This can be explained by the large simulation error during the destabilization period occurring at day 24.

V. Conclusions and perspectives

A distributed-parameter model for an anaerobic digester has been developed, identified and validated. This model is very useful to monitor and control, and may give some additional information to the uniformed-parameter model. In particular,

1. It gives a better understanding of what happens within the reactor;
2. It may be used as a diagnostic tool for process failures, as clogging for instance;
3. It may be used for sensor location studies as its structure allows to emphasize concentration gradients;
4. Hydrodynamic parameters can be regulated to optimize the process efficiency.

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