Modelling and identification of a Partial Differential Equation Model for an Anaerobic Wastewater Treatment Process

O. Schoefs[1], D. Dochain[2], H. Fibrianto[2] and J.P. Steyer[3]
[1]UTC, BP 60139, 60203 Compiègne, France
[2]CESAME, Université Catholique de Louvain, 4-6 av. G. Lemaître, 1348 Louvain-la-Neuve, Belgium
[3]LBE-INRA, avenue des étangs, 11 100 Narbonne, France

Abstract The objective of this paper is to present a partial differential equation (PDE) model for a fixed bed anaerobic digestion process. In practice, in fixed or fluidized bed reactors, liquid phase concentrations may often 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].
Keywords. fixed bed reactor, modelling, partial differential equations, convection-diffusion-reaction.

Introduction

In anaerobic digestion in fixed bed reactors, when working over a long period of time, clogging of the bioreactor can occur. 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 a large number of 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 PDE model may be useful to better describe what happens in the reactor, to study the influence of hydrodynamic conditions, to be used as part of a diagnosis tool for process failure such as clogging, and to implement advanced control strategies. The methodology follows three steps: transformation of a validated ordinary differential equation (ODE) model into a PDE model, parameter calibration by using steady-state data, and model validation under transient conditions.

Dynamical model of the fixed-bed anaerobic digester

The extension of the CSTR-type model developed and validated in [BER, 01] in order to account for the spatial concentration distribution gives the following convection-diffusion-reaction (CDR) model described by the following set of partial differential equations (PDE's)⊡

$$\frac{\partial X_1}{\partial t} = (\square_1 \square\square \cdot D) \cdot X_1 \tag{1}$$

$$\frac{\partial X_2}{\partial t} = (\square_2 \square\square \cdot D) \cdot X_2 \tag{2}$$

$$\frac{\partial Z}{\partial t} = \square u_1 \cdot \frac{\partial Z}{\partial z} + E_z \cdot \frac{\partial^2 Z}{\partial z^2} \tag{3}$$

$$\frac{\partial S_1}{\partial t} = \square u_1 \cdot \frac{\partial S_1}{\partial z} + E_z \cdot \frac{\partial^2 S_1}{\partial z^2} \square k_1 \cdot \square_1 \cdot X_1 \tag{4}$$

$$\frac{\partial S_2}{\partial t} = \square u_1 \cdot \frac{\partial S_2}{\partial z} + E_z \cdot \frac{\partial^2 S_2}{\partial z^2} + k_2 \cdot \square_1 \cdot X_1 \square k_3 \cdot \square_2 \cdot X_2 \tag{5}$$

$$\frac{\partial C}{\partial t} = \square u_1 \cdot \frac{\partial C}{\partial z} + E_z \cdot \frac{\partial^2 C}{\partial z^2} \square q_C + k_4 \cdot \square_1 \cdot X_1 + k_5 \cdot \square_2 \cdot X_2 \tag{6}$$

with $\mu_1 = \mu_{1max} \cdot \frac{S_1}{K'_{S1} \cdot X_1 + S_1}$ $\mu_2 = \mu_{2s} \cdot \frac{S_2}{K'_{S2} \cdot X_2 + S_2 + \frac{S_2^2}{K_{I2}}}$ (7)

$$q_C(z+dz) = q_C(z) + k_L a \cdot (A.dz) \cdot (C(z) + S_2(z) - Z(z) - K_H \cdot P_C(z)) \quad (8)$$

where $$P_C = \frac{\Phi(z) - \sqrt{\Phi(z)^2 - 4 \cdot K_H \cdot P_T(z) \cdot \left[C(z) + S_2(z) - Z(z) + \frac{q_C(z-dz)}{k_L a \cdot dV}\right]}}{2 \cdot K_H} \quad (9)$$

with $$P_T(z) = P_T + \rho \cdot g \cdot (H - z) \quad (10)$$

$$\Phi(z) = C(z) + S_2(z) - Z(z) + K_H \cdot P_T(z) + \frac{q_M(z) + q_C(z-dz)}{k_L a \cdot dV} \quad (11)$$

$$q_M(z+dz) = q_M(z) + k_6 \cdot \mu_2 \cdot X_2(z) \cdot A \cdot dz \quad (12)$$

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

In this model, A, u_L, E_z, S_1, S_2, X_1, X_2, μ_1 and μ_2, Z and C , Pc , P_T, q_C, q_M, K_b, D, a are the cross section area, the liquid velocity, the coefficient of axial dispersion, the organic substrate characterized by its chemical oxygen demand (COD), the volatile fatty acids (VFA), the acidogenic and methanogenic bacteria, the specific growth rates of acidogenesis and methanization, the total alkalinity and the total inorganic carbon, the carbon dioxide and the total pressure, the carbon dioxide and methane flow rates, an affinity constant, the dilution rate, and the fraction of bacteria in the liquid phase, 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} biokinetic parameters; $k_L a$ the liquid-gas transfer coefficient; K_H is the Henry's constant.

Remark : Note that a Contois-based relationship (instead of classical Monod or Haldane structures) has been introduced into the microbial growth kinetics. This choice is motivated by two arguments.

1) the choice of kinetic models for the specific growth rates that only depend on the limiting substrate concentrations leads to model for which the only admissible steady-state profile is with no biomass ($X_1 = X_2 = 0$)(see equations (1) and (2)). The introduction of the term dependent on the biomass concentration in the specific growth rate model allows to circumvent this problem and generate other steady-states, i.e. non-zero biomass concentrations.
2) 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 : this is the typically the situation experimentally observed.

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

Identification of the CDR model

The hydrodynamic parameters were identified by using the total alkalinity (equation (3)) data [BER, 01]. Due to the high inlet liquid flow rate, the model is not very sensitive to the hydrodynamic parameters so that accurate parameter calibration is difficult to obtain. The best results have been obtained with Ez equal to 1. The mean value of the Peclet number ($Pe = u_l H/Ez$) is 20, which corresponds to a highly dispersed plug flow behaviour.

Since a Contois-based Kinetics was introduced in the formulation 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: $K'_{S1} = \frac{K_{S1}}{\overline{X}_1}$ and $K'_{S2} = \frac{K_{S2}}{\overline{X}_2}$ where $\overline{X}_1$ and $\overline{X}_2$ denotes the mean values of the corresponding biomass. Due to the influence of this change on the model calibration, k_2, k_3, k_5 and k_6 had to be re-identified using steady-state data. Values of parameters for the two models are summarized in Table 1.

Table 1. Values of parameters and errors for both models

Parameter	Value - CSTR -	Value - CDR -	**State variable**	Error (%) - CSTR -	Error (%) - CDR -
μ_{1max} (1/d)	1.2	1.2	**COD**	34.02	6.99
K_{S1} (g/L) or K'_{S1} (g S_1/g VSS)	7.1	50.5	**VFA**	13.71	13.76
μ_{2s}	0.74	0.74	**Z**	4.58	4.75
K_{S2} (g/L) or K'_{S2} (g S_2/g VSS)	9.28	16.6	**C**	6.64	6.85
K_{I2} (mmol/L)	256	256	**Q_{CO2}**	6.45	4.01
α	0.5	0.5	**Q_{CH4}**	2.91	2.16
k_La (1/d)	19.8	19.8	**Q_{tot}**	3.53	2.38
K_H (mol/(L.atm))	16	16	**pH**	0.25	0.29
k_1 (g/g)	42.14	42.14	**VSS**	9.49	16.22
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 CDR model are presented in Figures 1, 2 and 3. Space derivatives were approximated using the finite difference method and ten nodes were considered. Qualitatively, the CDR model is able to describe experimental data as well as the CSTR model with the gain of a better description of the biomass concentration. Simulation curves of the biomass profiles within the reactor show the presence of a concentration gradient (see Fig. 3), and that clogging is more likely to occur at the reactor inlet. This is confirmed by experimental clogging observations [HAR, 02].

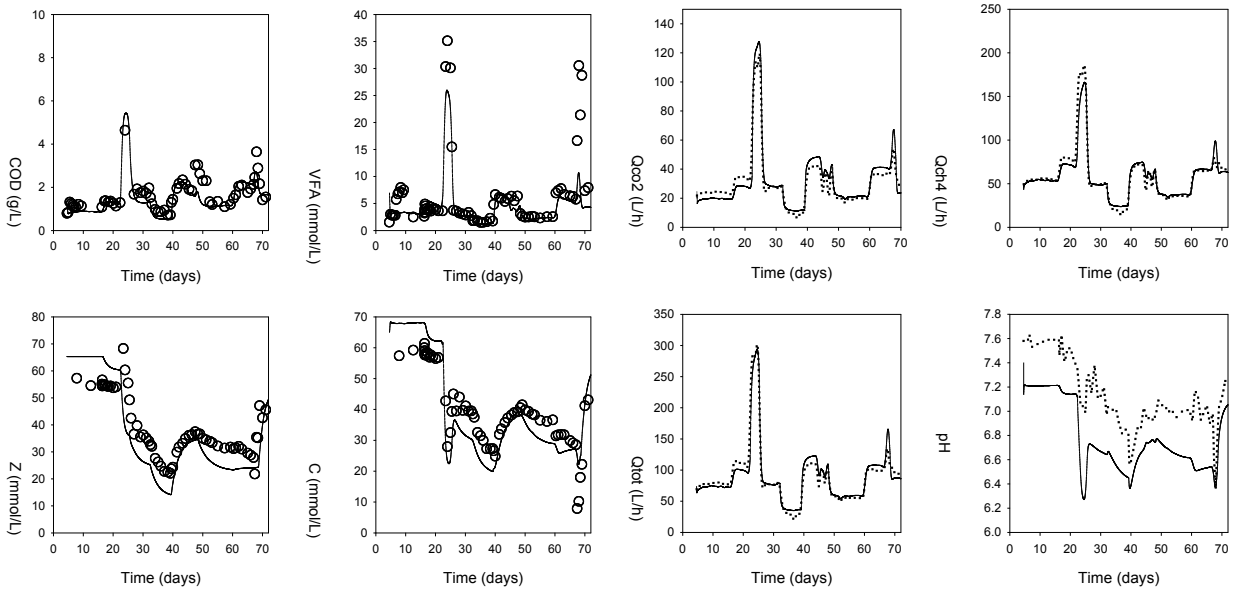

Fig. 1 Measured (o) and simulated (——) data for COD, VFA, alkalinity and total inorganic carbon (left) and for gaseous flow rates and pH (right).

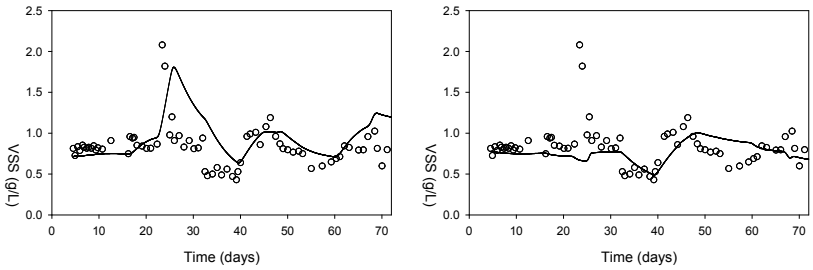

Fig. 2 Measured (○) and simulated (——) data for VSS (left: CDR; right: CSTR)

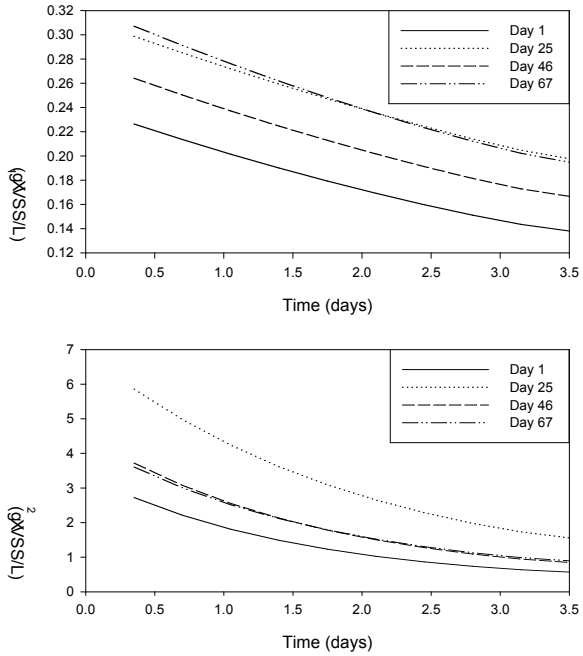

Figure 3. Simulation of the biomass profiles within the reactor.

The following quadratic criterion was used to compare the performance of both models,:

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

where $\hat{y}(\theta)$ and $y(\theta)$ denotes the predicted and the actual value of the variable y at time θ. Errors for each state variable in both models are calculated (Table 1). Simulation errors are similar for all state variables except for COD and VSS. Error on COD simulation curve was drastically reduced (from 34% to 7%) due to a better description of the beginning of the experiment, and of the destabilization phase occurring at day 24. Surprisingly, even if the dynamics of the biomass output is clearly better described by the CDR model, the simulation error is increased (from 9.5% to 16.2%). This can be explained by the recurrent five-day delay observed in the simulation curve.

References

[BER, 01] O. Bernard, Z. Hadj-Sadok, D. Dochain, A. Genovesi, and J.-P. Steyer, "Dynamical Model Development and Parameter Identification for an Anaerobic Wastewater Treatment Process," *Biotechnol. Bioeng.*, vol. 75, 2001, pp. 424-438.

[HAR, 02] J. Harmand, F. Miens, T. Conte, P. Gras, P. Buffière, and J.-P. Steyer, "Model Based Prediction of the Clogging of an Anaerobic Fixed Bed Reactor," *Water Sci. Technol.*, vol. 45, 2002, 255-262.

[KIE, 97] G. Kiely, G. Tayfur, C. Dolan, and K. Tanji, "Physical and Mathematical Modelling of Anaerobic Digestion of Organic Wastes," *Water Res.*, vol. 31, 1997, pp. 534-540.