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Hydrodynamic Model of an Anaerobic Reactor

Maha Hmissi^{*,**}, Jérôme Harmand^{**} and Hedi Shayeb^{*}

ABSTRACT

In this work, we focus on the anaerobic digestion model no 1 proposed by I.W.A. working group (Batstone et al. 2002) as a basis for the development of a comprehensive distributed parameter model, which combined ADM1's kinetics of biomass growth and substrate transformation with axial dispersion material balances. Then we present a two-step procedure to validate the simulations using the software COMSOL MULTIPHYSICS to resolve the complex system of PDEs. It is based on situations in which solutions must be approached from those of the homogeneous system. Then we study the influence of certain operational parameters such as residence time on the performance of the reactor.

Keywords: ADM1, Axial dispersion, PDE, Comsol Multiphysics.

1. INTRODUCTION

Generally in an anaerobic treatment, the reactor performance is influenced by the hydrodynamic behavior since it has direct impact on the extent of contact between the substrate and the microorganisms, and also because it can influence the rates of biological reactions through changes in the rate of mass transfer and in the distribution of reactions along the reactor [8].

Various researchers have carried out studies to understand the hydrodynamic behaviour of anaerobic reactors [1], several performance-prediction models have been proposed, dealing with kinetic expressions that describe the degradation and the production of organic and inorganic substrates inside the reactor. In some cases, these models have been coupled with the hydrodynamic description of the process to take into account the variability existing among the various configurations that certainly affect the overall performances of the treatment [7].

According to [5], hydrodynamics plays an important role in the study of anaerobic reactors, because it can influence the rates of biological reactions through changes in the rate of mass transfer and in the distribution of reactions along the reactor.

In [11-19], the authors proved that the operating conditions are suitable for the formation of biofilm granules in the UASB reactors but they also lead to the existence of significant substrate and biomass gradients in the sludge bed, which have a profound influence on long-term reactor performance and stability during shock loads. This experiment focusses on the sludge dynamics along the reactor height.

According to [10-16], hydrodynamics were studied experimentally in a flushed bed reactor by interpreting the Residence Time Distribution curves.

According to Fick's law, the rate of diffusion of a substance C in a reactive medium is proportional to the negative of the concentration gradient of C . In any tubular reactor, either empty or packed, reactant depletion

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and nonuniform flow velocity profiles give rise to concentration gradient, and hence diffusion, in axial direction. A reactor model which accurately reflects these phenomena is difficult to derive, and even more to analyze. What is often done instead is to model the reactor making the following two assumptions:

The process fluid moves through the reactor at a uniform velocity U equal to the mean velocity of the fluid in the reactor being modeled.

Dispersion occurs only in the axial direction. The extent of the dispersion is sufficient to account for the combined effects of all dispersive phenomena (molecular and turbulent mixing, and non-uniform velocities) in the real reactor. This representation of a flow reactor is termed the dispersed plug flow model [15]. Some recent control methods are discussed in [20-25].

Hydrodynamic behaviour is usually described using two ideal flow patterns, i.e. plug flow and perfectly mixed flow, or their combinations. Falling between the two ideal flow patterns, the axial dispersion model allows backmixing to be characterised by equations derived by analogy with Fick's-Law equation [3].

The Anaerobic digestion model no. 1 (ADM1) was proposed by the International Water Association task group on anaerobic digestion [2], it uses the assumption of ideal mixing. The ADM1 is a structured mathematical model with 32 dynamic state concentration variables and involves 19 biochemical rate processes: The set of differential equations (DE) of the ADM1 model are as follows: 10 (DE) to model the evolution of soluble matter concentrations in liquid phase and two (DE) to model inorganic carbon (IC) and inorganic nitrogen (IN) levels in liquid phase. Twelve (DE) others depict the dynamic behaviour of particulate matter and biomass concentrations in liquid phase; two (DE) to model cations and anions levels in liquid phase and an additional six (DE) for acid-base reactions in order to determine the pH of effluent and to calculate ionized forms of VFA, free ammonia nitrogen and carbon-dioxide concentrations [2].

In the present work, the kinetic model (ADM1) is coupled with the hydrodynamic model (Axial Dispersion Model) [4] and coded using the software COMSOL Multiphysics. In this paper we propose the model equations and a procedure to validate the code used to simulate them. This procedure based on the comparison of steady state qualitative properties of the ADM1 and simulations of its spatially-distributed counterpart parameterized in such a way these simulations should coincide. Then we present the results of the validation of the spatialized ADM1 while finally we present preliminary results about its specific behavior.

2. MODEL IMPLEMENTATION

2.1. Liquid phase

The distributed parameter model takes into account the same dynamic state than the ADM1 for a completely stirred tank reactor (CSTR), all processes (biochemical as well as physicochemical) inside the reactor being considered to depend only on the vertical axis of the reactor (distance z from input, z varies from 0 to H) and time t . The spatial distribution of the concentration of any component C_i (soluble or suspended) along the reactor height z can be expressed on the basis of the dispersed plug flow concept [12-19] using the following equation that was solved under steady-state conditions, with the Danckwert boundary conditions:

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial z} \left(D_i(z,t) \frac{\partial C_i(z,t)}{\partial z} - \frac{\partial}{\partial z} (U_i(z,t) C_i(z,t)) + r_i \right) \quad (1)$$

where D_i is the dispersion coefficient, U_i is the upflow velocity, z (z varies from 0 to H) is the axial position and t is the time. The first term in the right part of Eq. 1 characterises the dispersive term. The second term determines a convective transport of component C_i in the vertical direction. The third is the net biotransformation rate for component C_i , respectively.

The Danckwerts boundary conditions (Danckwerts, 1953) are:

$$D_i(z,t) \frac{\partial C_i}{\partial z} = U_i(z,t) (C_{i(z=0)} - C_{i,in}), z = 0$$

$$\frac{\partial C_i}{\partial z} = 0, z = H \quad (2)$$

2.2. Gaseous phase

The gaseous components (methane, hydrogen, carbon dioxide) are treated in the model as solutes and the transfer to the gas phase is considered as an ideally mixed medium [12].

The dispersion and convective transport of bubbles in the liquid are considered negligible in comparison with the gas transfer rate. The following equation was used to describe the mass transfer from the liquid to gas phase [19].

$$\frac{\partial S_{gas}(z,t)}{\partial t} = \frac{V_{liq}}{V_{gas}} r_T(z,t) - \frac{1}{V_{gas}} \frac{\partial}{\partial z} (q_{gas}(z,t) S_{gas}(z,t)) \quad (3)$$

q_{gas} is the volumetric flow rate of biogas, which is defined as [12]:

$$q_{gas} = \sum V_{m,gas} \int_0^H M_{T,i} dz \quad (4)$$

while V_m is the specific molar volume of gas under given temperature and equal to:

$$V_{m,gas} = \frac{RT}{P_{atm} - \rho_{gas,H2O}} V_{liq} \quad (5)$$

The boundary conditions of the gas components are: $S_{gas,j} = 0$ at $z = 0$ and $\frac{\partial S_{gas,j}}{\partial t} = 0$ at $z = H$. The reactor is viewed as a single tube with a dispersive plug flow, which includes both advection and reaction, in addition to axial dispersion. The parameter taking into account the mixing in the reactor is the Peclet number in the axial dispersion model [17] which is defined as:

$$Pe = \frac{U_i H}{D_i} = \frac{\text{Convective Flow}}{\text{Dispersive Flow}} \quad (6)$$

A low Peclet number means a large dispersion. On the other hand, a reactor with plug flow has a high Peclet number [15] and Convective Flow Dispersive Flow.

3. COMPARISON BETWEEN AN ADM1 (CSTR) AND A DISTRIBUTED PARAMETER MODEL: BENCHMARKING

The aim of this part is to introduce spatialization on the ADM1. This study uses model parameters and operating conditions employed in ADM1 benchmark simulations [18] for comparison of the distributed parameter and an ADM1 (CSTR) models. At the startup of each simulation, steady-state outputs of the ADM1 benchmark simulations (the homogenous version of the ADM1) were used as initial values for the distributed model.

To evaluate the spatial version of the ADM1, two kind of numerical experiments were realized at steady state and in dynamic. First it is verified at equilibrium that when Pe is small, the simulations obtained

with the spatially version of the ADM1 are close to the predictions of the homogenous ADM1. Then still at equilibrium and with a small Peclet, we compare the qualitative behaviors of both models in increasing gradually the input flow rate and observing if the washouts of different species are observed for the same flow rates and in the same order.

Finally, still with small Pe , we compare outputs of both models in dynamics.

3.1. Peclet Number

In this part, we try to validate the simulator in comparing the behaviour of the spatialized system when it is parameterized in such a way it should behave as the homogeneous system.

The two models were compared by analyzing the concentrations of: Total COD, Volatil fatty acids (VFA), Biomass, Inorganic nitrogen (SIN), production of biogas (q_{gas}), %CH₄ and soluble COD (S).

For the distributed parameter model we took a very small Peclet number ($Pe = 10^{-5}$) i.e the dispersion coefficient $Dz \rightarrow \infty$ (perfect mixing conditions) then we compared the outputs of the two models.

The distributed parameter model introduced in Comsolmultiphysics reproduced adequately the outputs of ADM1 (CSTR) with a little difference between the pourcentage of methane Figure 1.

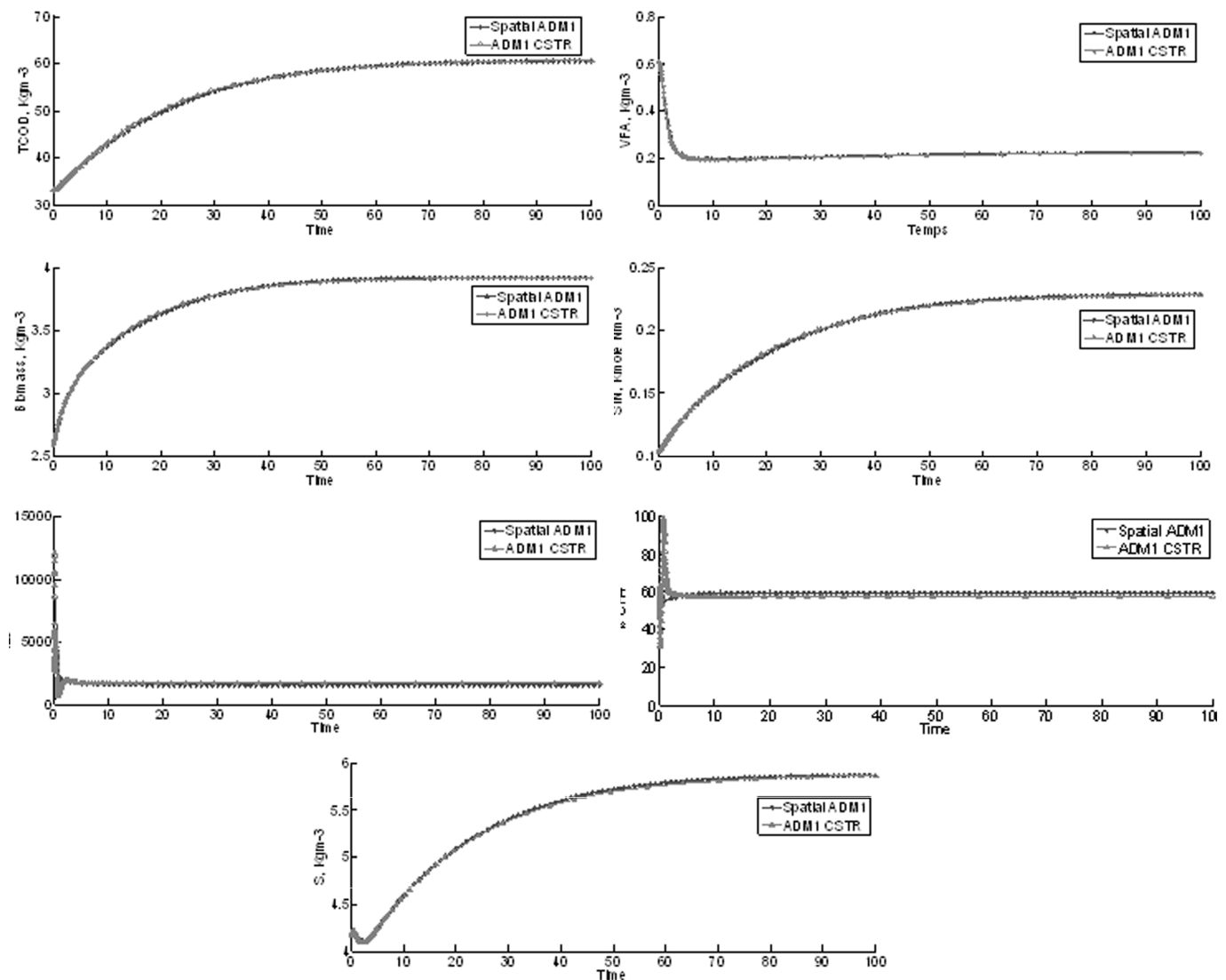


Figure 1: Comparison between an ADM1 (CSTR) and a distributed parameter model: Benchmarking results for CODT, VFA, Biomass, SIN, q_{gas} , %CH₄ and Soluble COD

Correct benchmarking results were achieved using steady-state data, as for example shown in Figure 1. The ADM1 (CSTR) model outputs and the outputs of the ‘implementation developed’ (Distributed parameter model) do not differ significantly. The lower means relative error in an order of magnitude of 0.03% indicates the numerical accuracy in generating the output for both model implementations.

3.2. Dilution

After verifying that we have obtained the same results for the two models (ADM1 CSTR and spatial ADM1) at equilibrium with a small Pe , we try to establish if the qualitative behaviour of the two models is the same Figure (2-3).

Always at equilibrium, we increase gradually the inflow rate to see the successive washout of biomasses. Various simulations were performed at different dilution rates D ($D = U/L$) while increasing each time the flow velocity U for an ADM1 (CSTR) and a spatial ADM1. By increasing the flow rate we found that biomasses behave the same way for both models; the concentrations of Carbohydrates X_{ch} and lipids X_{li} increase with increasing of the dilution rate. Furthermore, when the dilution rate increases, it is observed that biomasses of sugars X_{su} , amino acids X_{aa} , fatty acids X_{fa} , propionates X_{pro} , and acetate X_{ac} begin to decrease slightly.

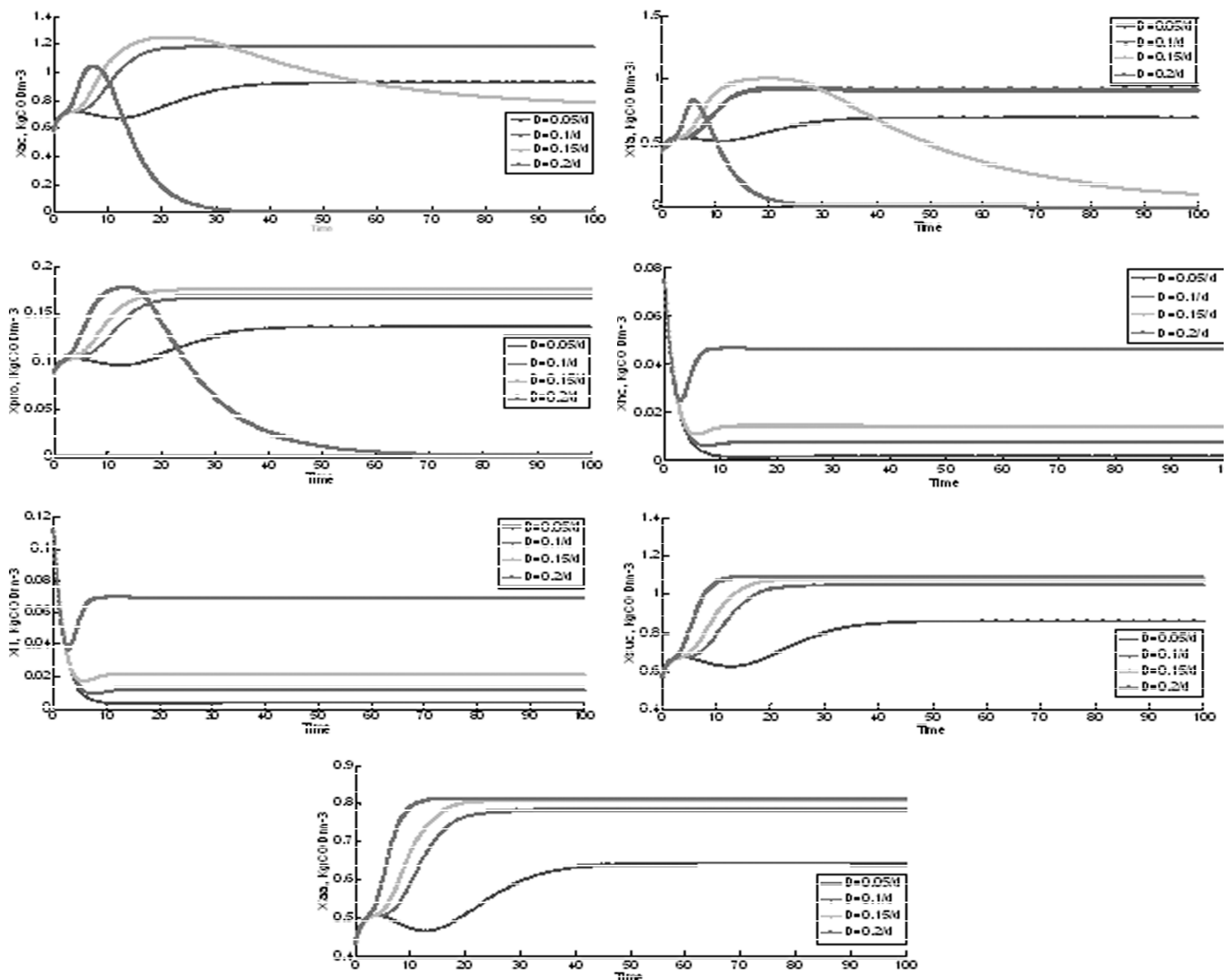


Figure 2: ComsolTemporel profile along the reactor for the distributed parameter model

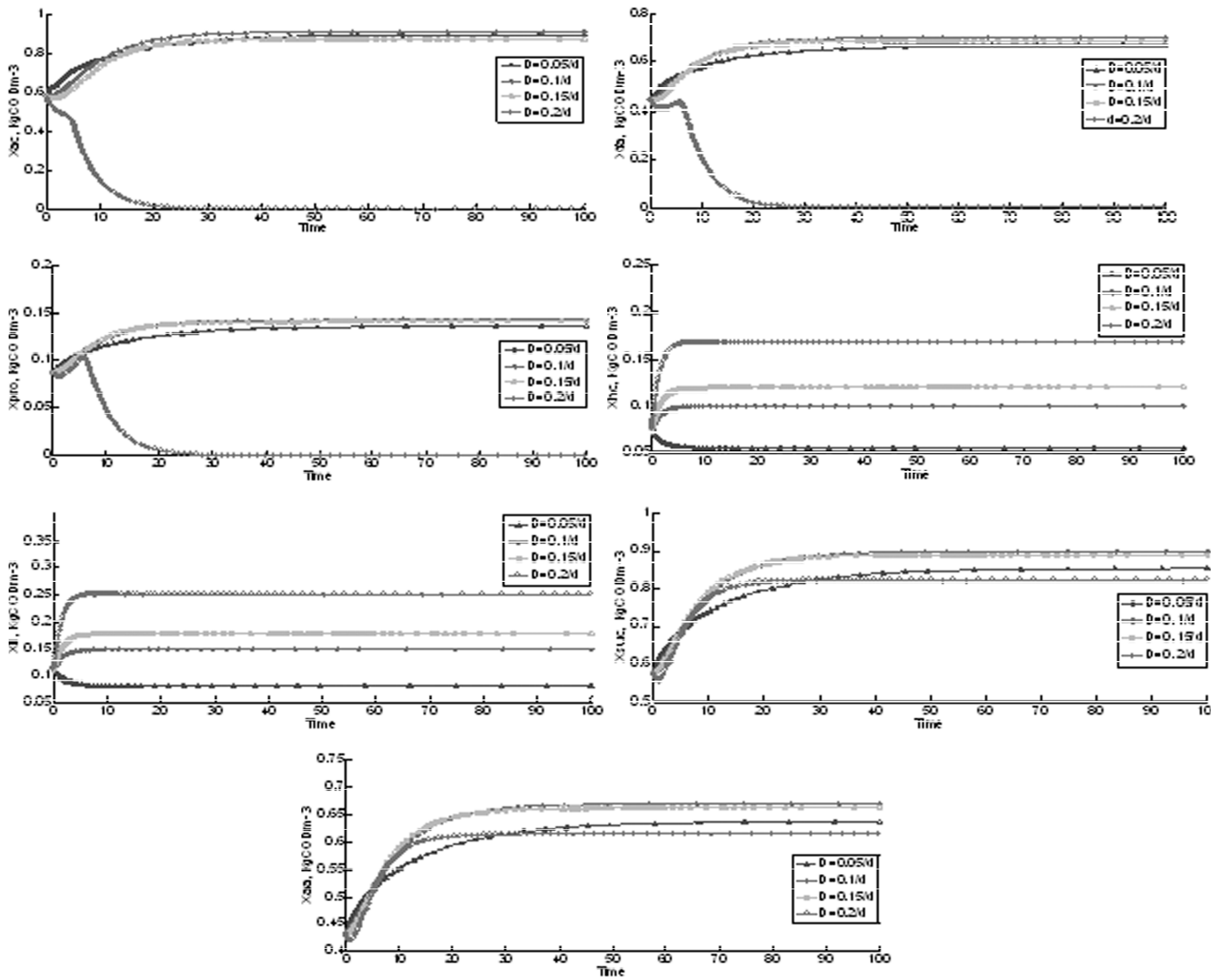


Figure 3: Temporal profile for the ADM1 (CSTR)

The biomasses X_{fa} , X_{pro} and X_{ac} successively disappear for the dilution $D=0.2/\text{day}$ for the two models. As a consequence, it is noted that the same biomasses in the two models reach the washout at identical hydraulic residence times.

It is concluded that both models have the same qualitative behaviour Figure (2-3) with respect to these important properties.

4. COMSOL RESULTS: COMPARISON BETWEEN THE PRODUCTION OF BIOGAS FOR AN HOMOGENOUS AND A DISTRIBUTED ADM1 MODEL

In this section, we present preliminary results about the study of the proposed spatially-distributed ADM1. Figure 4 presents how the biogas production q_{gas} at steady state changes with the dilution rate D ($D = U/L$). For all HRT simulated, the biogas production first increases with the dilution rate to reach a maximum, and then decreases. At high dilution rate the production is very low due to the washout of microorganisms Figure 5. In any case, the qualitative behavior of the biogas production rate exhibit the same shape for the two models. In fact, an increase in the dilution rate D resulted in a modification of both the composition of the microorganisms in the system and the concentrations of all state variables. As D increased, the concentration of the biomass first increased rapidly and then fell down while the

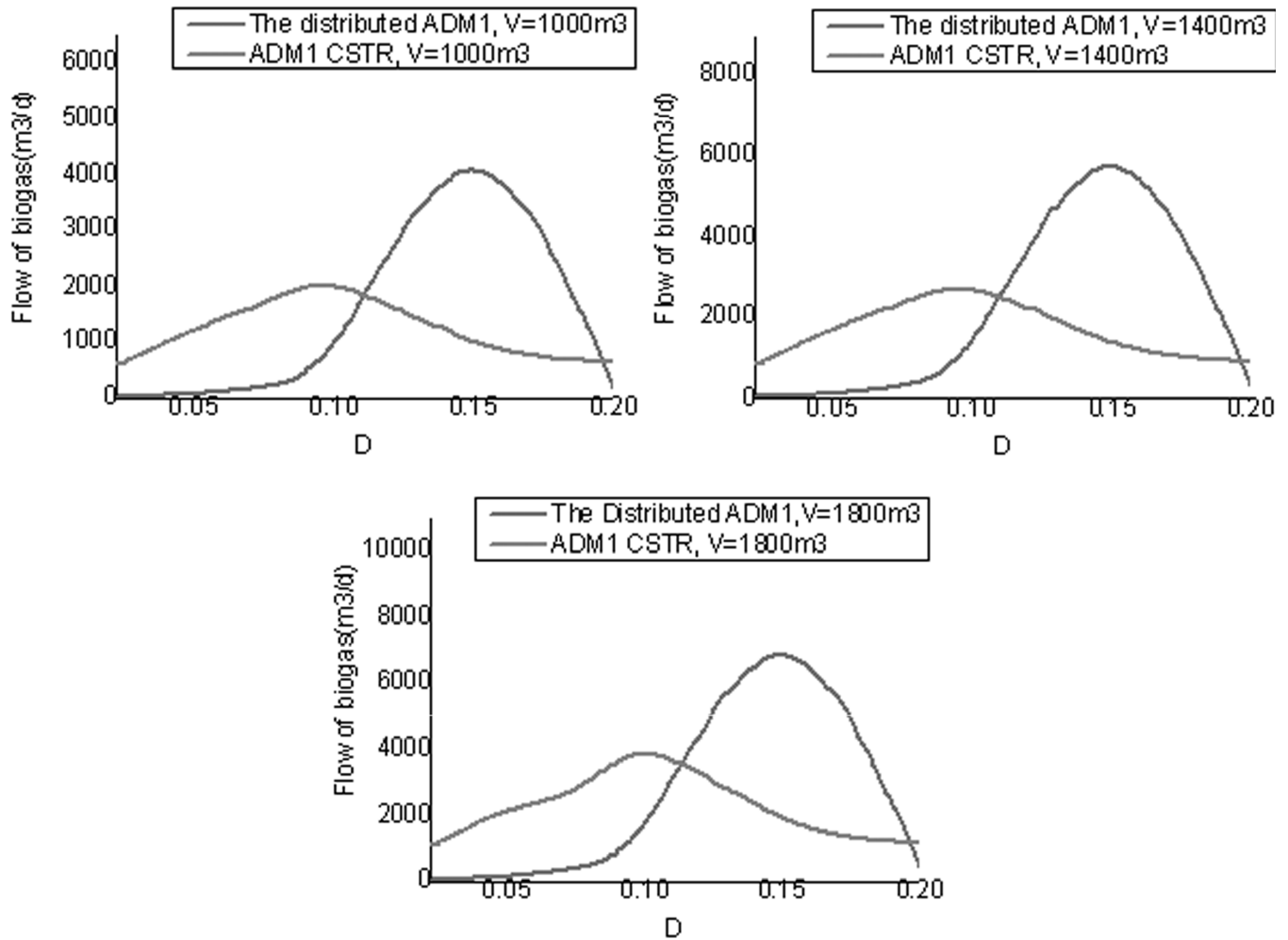


Figure 4: Comparison between the production of biogas for the homogenous ADM1 and a distributed model

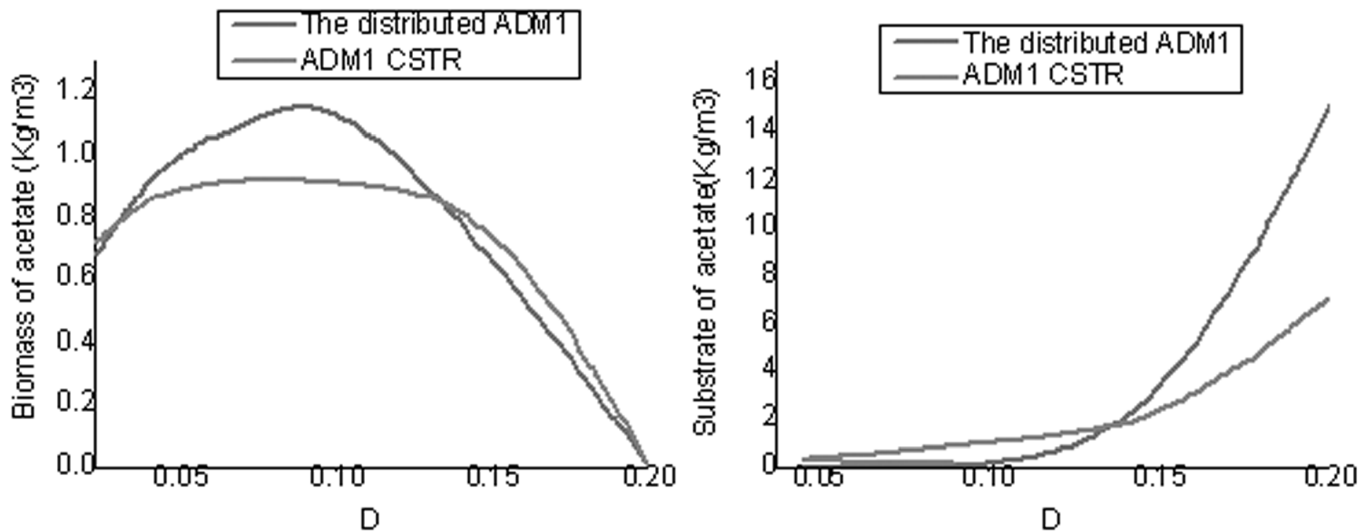


Figure 5: The effect on the biomass as D varies (V=1400m³)

methanogenic biomass approached extinction. Figure (4) presents a comparison between the biogas production for a homogenous ADM1 (CSTR) and the distributed parameter model. For the same volume of the reactor the maximum rate of biogas for a distributed model is higher than the ADM1 CSTR. The flow of biogas rate increases with an increase in the velocity and it increase with the increasing of the volume of

the reactor. The comparison showed that the distributed model was better suited for maximizing the production of biogas.

A comparison of effluent concentrations predicted by ADM1 (CSTR) and a distributed ADM1 is shown in Figure. 5. As the result, ADM1 distributed output for effluent substrate of acetate was lower than this of ADM1 CSTR. Consequently, the spatial ADM1 predicted higher effluent biogas flow rate Figure. 4. This trend was in agreement with results obtained in [19]. The responses of both models to increased velocity U were similar, the substrate of acetate was low which can be attributed to the increase of biomass in the reactor, and then it increased due to the washout of biomass.

The simulated concentration of acetate substrate in the reactor effluent of the distributed ADM1 was less than those predicted by ADM1 Figure. 5. This can be explained by the fact that in ADM1 biodegradation rates were the same at all reactor positions, while in ADM1d the rates were position dependent. The Monod-like kinetic equations, which were used to describe biotransformations in ADM1d, resulted in higher degradation rates predicted at the bottom the reactor, where substrate concentrations were the highest. Consequently, an overall volumetric rate of biodegradation was higher in ADM1d than in ADM1 thus resulting in lower effluent concentrations of acetate substrate.

5. CONCLUSIONS

In this study, Anaerobic Digestion Model No. 1 was used as a basis for the development of a comprehensive distributed parameter model. We used the software Comsol Multiphysics as a tool for the resolution of PDEs. To verify the applicability of Comsol Multiphysics we used two procedures. At the equilibrium when Pe is small, we found the same results for the two models (ADM1 CSTR and spatial ADM1). We also studied the influence of dilution rate on biomass for both models that have the same qualitative behavior while increasing the dilution rate. The capacity of a spatial ADM1 for predicting spatial distribution of state variables can be very useful in developing a systematic approach for the design and the optimization of anaerobic reactors.

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NOTE

1. <http://project.inria.fr/treasure/>

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