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# Novel approaches to modeling dry anaerobic digestion by considering water porosity evolution

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**Abstract:** Our previous findings revealed the distribution and evolution of three different pore water porosity types (microscopic, mesoscopic and macroscopic porosities) during dry anaerobic digestion (D-AD). Two novel and different models considering this phenomenon were developed. The first one combined the AM2 biochemical model with saturated Mobile-Immobile water model (AM2-MIM). The model considered the interactions of mass transfer between mobile phase (macroporosity) and immobile phase (microporosity + mesoporosity). The second model coupled this new model with a biofilm diffusion model to consider separately microporosity and mesoporosity (AM2-MIM+Biofilm), simulating the diffusion and the transformation of hydrolyzed substrates within the biofilm (mesoporosity). Both models allow a better understanding of the microbiological and hydrodynamic phenomena during D-AD processes.

**Keywords:** Mathematical modeling; AM2; Porosity

## Introduction

The dry anaerobic digestion (D-AD) with operational Total Solids higher than 15% is less common in industrial application but seems to be more efficient in the digestion of high solid content feedstock like straw, livestock manure and corn silage (André et al., 2018). However, the lack of knowledge of D-AD processes has always been the scientific hurdle for a larger deployment of this technology. Since digestate of D-AD is very pasty or even solid, the agitation for a sound homogenization in the reactor is difficult, which causes local accumulation of inhibitors like ammoniac and VFA and lead to the dysfunction of digesters. The insufficient agitation may limit the mass transfer of substrates and products. It also reduces the contact chance between the organic matter and the microbial consortium, slowing down the biogas production. It is also observed in the settlement of solid media during D-AD, meaning its mechanical (hydraulic) properties change. Hence, understanding the phenomena of the transfer and the hydrodynamic behaviors in D-AD reactors is critical to optimize the design and operation of processes.

Mathematical modeling can be therefore a useful tool for a better understanding of what is happening in digesters. Conversely to usual wet AD with CSTR, the biochemical model ADM1 is not sufficient to describe the whole SS-AD system. The introduction of other physical models such as interactions between different phases and phenomena of mass transfer is necessary to characterize the particular problems of SS-AD. Our previous study revealed the existence and the evolution of various types of pore water porosity in SS-AD digesters (i.e. microscopic, mesoscopic and macroscopic porosities, see Figure 1 and details in Hernández-Shek et al., 2020). The present study deals with the use of our previous findings about the water porosity evolution during SS-AD to develop different mathematical models simulating SS-AD processes: one coupling simplified biochemical model AM2 with Mobile-Immobile water model (see Coutu et al., 2022) and a second one coupling AM2 with a biofilm diffusion model inspired by the work of Coutu et al. (2022) and César and Silvio (2013).

## Material and Methods

The models work on the dry mesophilic anaerobic digestion of cattle manure (CM) in leach bed reactors. The first AM2-MIM model combines AM2, a simplified ADM1 model reducing four AD steps to three (Bernard et al., 2001), and the Mobile and Immobile water model (MIM), a hydrodynamics model simulating interaction between mobile and immobile phases. In this AM2-MIM model, only hydrolysis takes place in immobile phase (characterized by the sum of microscopic and mesoscopic porosities  $\theta_{im}$ ). All other biochemical reactions are considered only in the mobile region (described by the macroscopic porosity  $\theta_m$ , see Figure 2). The AM2-MIM model was applied at first on a single substrate (cattle manure) by neglecting the spatial variations in both two phases and therefore, becomes a 0-D model. Full development of the model equations is available in Coutu et al. (2022).

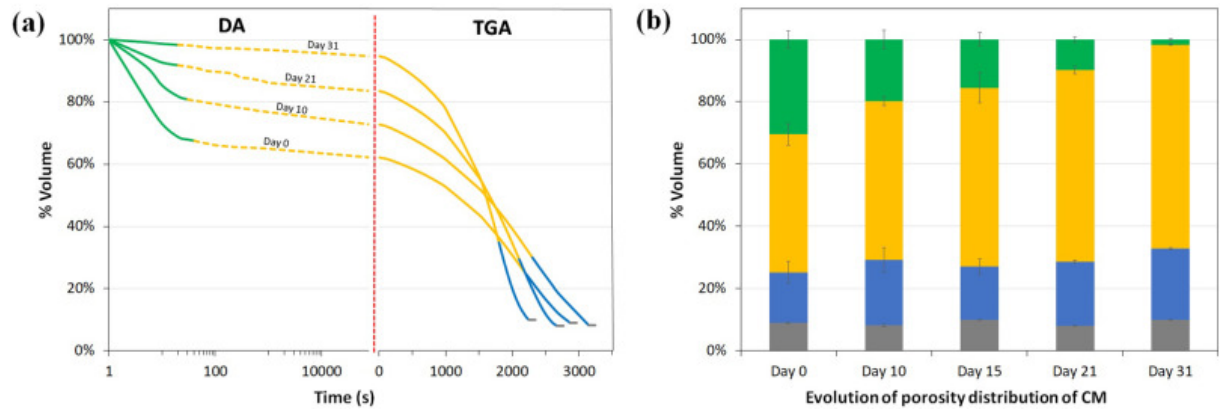
The second model was inspired by previous work and more based on the microbiological facts during the microbial degradation of organic matter. Inspired by previous work as mentioned above, the 3 different porosities (microscopic, mesoscopic and macroscopic porosities) are assumed to correspond respectively to the chemically bounded water region, the biofilm region and the free water region (see Figure 3). All the hydrolysis enzymatic reactions take place in chemically bounded water region (straw) and free water region (particulates) in which all concentrations of substrates are considered homogeneous. All the other reactions (acidogenesis and methanogenesis) occur in biofilm region whose evolution is described by the mesoporosity changes. The intermediate products ( $S_1$ ) resulting from hydrolysis have to diffuse within the biofilm adhered to the straw wall, so that the acidogens and methanogens ( $X_1$  and  $X_2$ ) are able to degrade them into VFA and eventually biogas ( $CO_2$  and  $CH_4$ ).

Both models consider the three types of pore water porosity evolution during the digestion. The ordinary partial equations (not shown here) were resolved by the function “ode15” and “pdepe” in MATLAB (MathWorks, Massachusetts, US). The optimization function “fmincon” was employed to identify the kinetic parameters of AM2-MIM models with a set of experimental data treating cattle manure. For AM2+Biofilm model, we used the kinetic parameters identified by AM2 modeling alone of the experimental results.

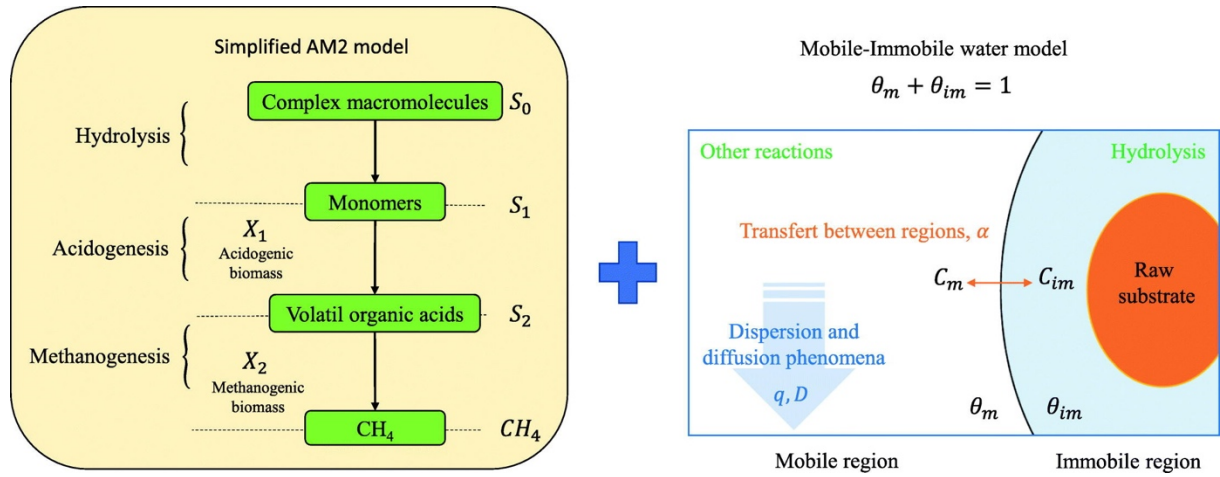
## Results and Conclusions

Figure 4 shows the simulation result of AM2-MIM model in a leach bed reactor treating cattle manure. The results are relatively satisfactory as compared to the experimental results. This confirms that the MIM model combined with AM2 could give a good description of the AD process in the reactors. This model provided a new understanding of hydrodynamics as well as an insight into the impact of macroporosity and microporosity evolution on D-AD.

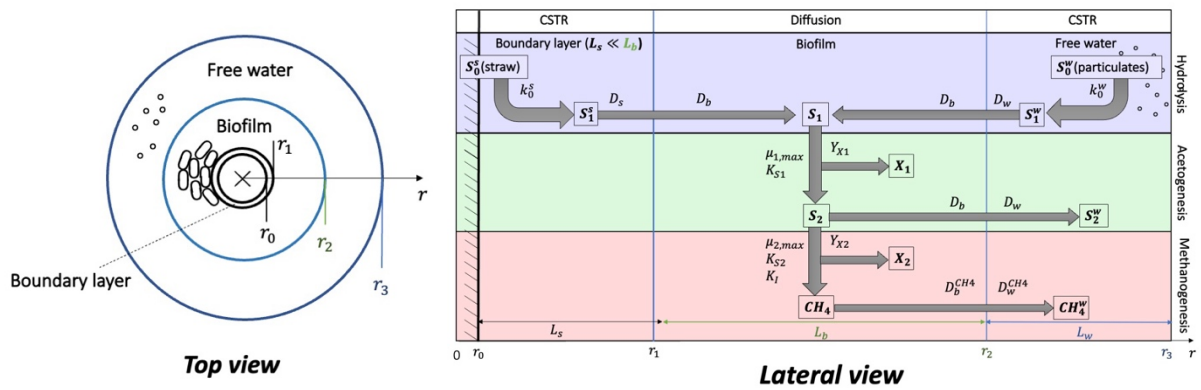
When it comes to the second model dealing with AM2+biofilm diffusion, it is shown in Figure 5 that the diffusion of the substrates within the biofilm causes significant uneven distribution of acidogenesis biomass and thus gives rise to an uneven production of VFA and  $CH_4$  within the biofilm. This novel AM2+biofilm model, even though pending further improvement, helps a better understanding of the microbiological phenomenon on a microscopic scale. Further research would be put in how to, by creating a spatial distribution, integrating the hydrodynamic behavior of water into the model to simulate the circulation of percolate in the solid mass.



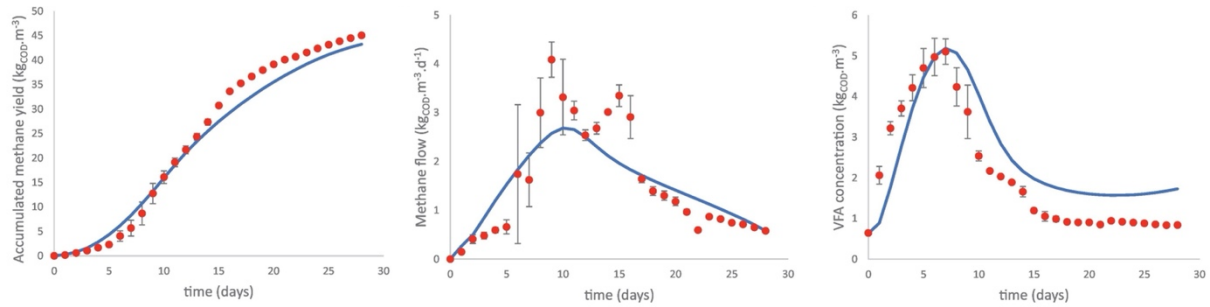
**Figure 1** (a) Water retention curves for cattle manure (CM) treated in 60 L Leach-bed reactors. (b) Porosity distribution evolution of CM during AD process (Hernández-Shek et al., 2020).



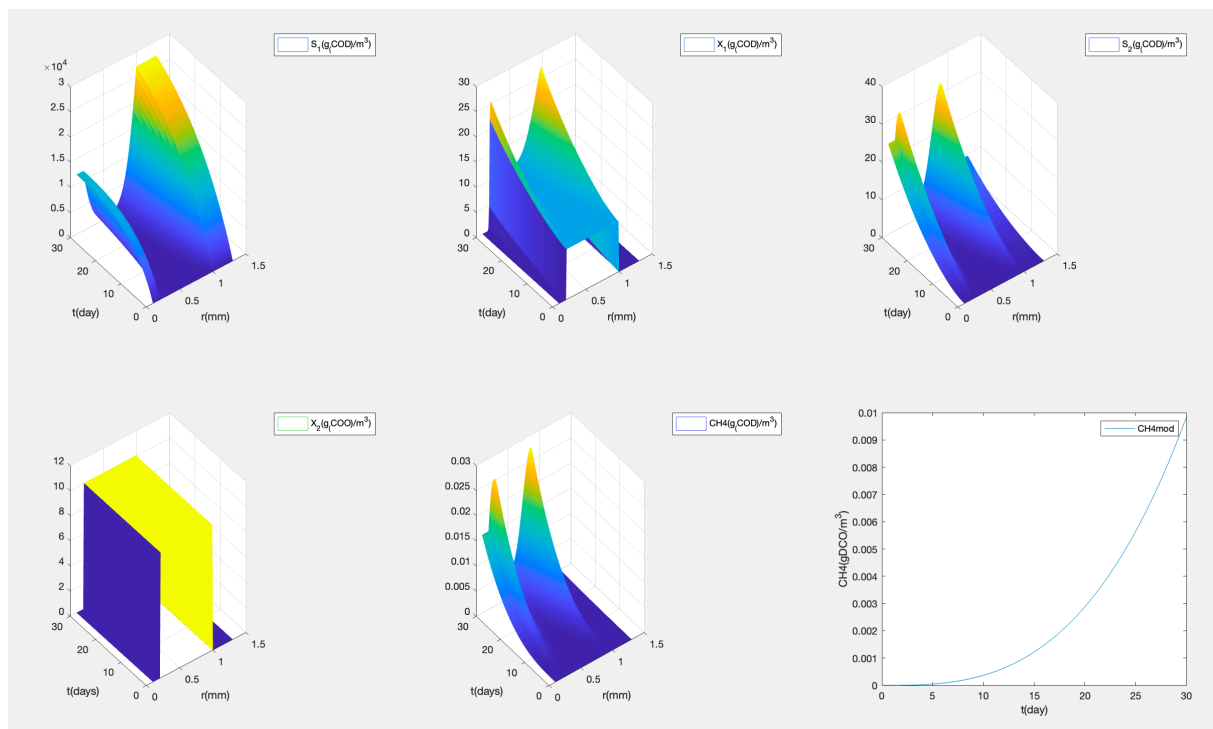
**Figure 2** Schematic representation of the model AM2 + MIM (Coutu et al., 2022).



**Figure 3** Schematic representation of the model AM2 + biofilm.



**Figure 4** AM2+MIM modeled results (curves) vs experimental observation (points) (Coutu et al., 2022).



**Figure 5** Spatial distribution of different parameters ( $S_1$ ,  $X_1$ ,  $S_2$ ,  $X_2$  and  $CH_4$  production) simulated by AM2+Biofilm model.

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