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Modelling of an anaerobic plug-flow reactor. Process analysis and evaluation approaches with non-ideal mixing considerations

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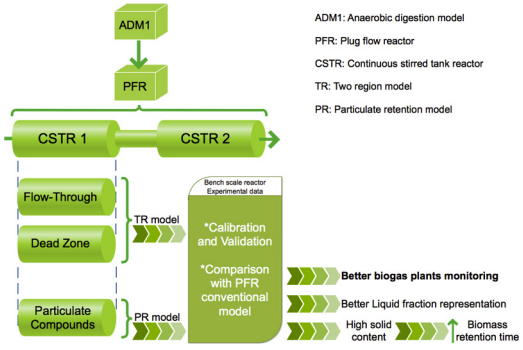
GRAPHICAL ABSTRACT



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ABSTRACT

This study shows the implementation of the Anaerobic Digestion Model (ADM1) in an anaerobic plug-flow reactor (PFR) with two approaches based on the use of consecutive continuous stirred tank reactors (CSTR) connected in serie for considering non-ideal mixing. The two-region (TR) model splits each CSTR into two regions, while the particulate retention (PR) model adds a retention parameter. The models were calibrated and validated based on experimental data from a bench-scale reactor treating cow manure. The PFR conventional model slightly outperformed the non-ideal mixing approaches. However, the PR model showed an increase in biomass retention time treating high solid content substrate. Biogas production was not sensitive to variations of the mixing parameters. The liquid fraction content was better represented by the PR model than the PFR and TR models. The study shows how reactor modelling is useful for monitoring and supervising biogas plants.

1. Introduction

Anaerobic digestion (AD) is a well known technology. In the last decades there has been a steady increase in the total number of AD plants, as well as in the total capacity of electricity produced from biogas (Vasco-Correa et al., 2017). In Chile, AD has started to pick up in the last decade and there are around 75 full scale digesters currently operating (Avila et al., 2016). CSTRs working at (semi)continuous mode have been widely preferred. However, PFRs are increasingly implemented, especially for livestock manure treatment (Batstone et al., 2015). PFRs present several advantages in comparison to CSTRs, such as an appropriate use of the working volume, higher capacity for

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overloads, more protection against acidification and the generation of concentration profiles along the reactor. On the other hand, PFRs may undergo instabilities due, for example, to the cascade acidification that results from the low local retention time of each section of the reactor. Few full-scale applications of PFRs have been reported, most of them associated with the treatment of cow manure in the USA (Li et al., 2014; St-Pierre and Wright, 2014, 2013).

Nowadays, mathematical modelling of biochemical processes is recognized as very important for process analysis, control and optimization. Proper modelling leads to a deeper insight into the process, evaluating different scenarios and hypotheses, having a virtual plant for the assessment and training, and achieving process control and better experimental designs (Batstone et al., 2015). Also, it helps to minimize the experimental work, which means money saving, time reduction and less risk. The ADM1 developed by International Water Association (IWA) is the most widely recognized and popular mathematical model for AD process, which has been extensively used in modelling research (Batstone et al., 2006). Nevertheless, there is insufficient literature associated with the modelling of PFRs due to their recent implementation. Unlike a CSTR, in a PFR a specific compound concentration will depend on time and position along the reactor. Therefore, theoretically, the modelling is more complex in a PFR than in a CSTR. Moreover, when the types of substrate that are fed into the reactor are given, perfect mixing or homogeneity will rarely be achieved (Capela et al., 2009). The modelling of a digester treating semi-solid waste has been recognized as an important issue that needs to be addressed (Liotta et al., 2015b). PFRs have been mainly used for treating high solid content substrates. Therefore, mixing must become critical since keeping a proper agitation will be difficult to achieve. It has been reported in the literature that PFRs have been modelled by using partial differential equations (PDE) (Liotta et al., 2015a), by ordinary differential equation (ODE), using CSTRs connected in series so the PDEs are avoided (Bensmann et al., 2013; Ghaniyari-Benis et al., 2010), and by using computational fluid dynamics (CFD) (Wu, 2012).

There is a lack of literature dealing with PFR and also about modelling approaches. The aim of this study was to develop a mathematical model based on the ADM1 for an anaerobic PFR. Two different approaches to considering reaction media heterogeneity were implemented and tested. This article is structured in three main sections: model development, numerical simulation, and model calibration/validation with experimental data from a pilot-scale reactor.

2. Materials and methods

2.1. ADM1 adjustment

The ADM1 model with the modifications proposed by Rosen and Jeppsson (2006) was used. The parameters were kept as suggested by the ADM1 report. The composite concentration (Xc) was setted equal to zero, so the particulate carbohydrates, proteins, lipids, soluble monosaccharides, amino acids, volatile acids and inerts were the input conditions to the ADM1 model, according to the methodology proposed by Kleerebezem and Van Loosdrecht (2006). The elimination of the disintegration step originally considered in the ADM1 has been lately suggested as necessary due to all the disadvantages of the two-hydrolysis step approach, especially for sewage sludge (Batstone et al., 2015). The temperature effect on the hydrolysis reaction was added in an explicit way to the model by using the Cardinal Temperature Model (CTM) (Donoso-Bravo et al., 2013a,b). The models were implemented and solved in Matlab®2015b by using the toolbox ode15s.

2.2. The PFR model

A PFR can be classically represented as an infinite number of CSTR reactors connected in series. Therefore, the coupling of several CSTRs was the chosen global approach used in this study. The ADM1 model was then solved for each CSTR where the output of the first one corresponds to the inlet and conditions of the following one, and so on. Due to the intrinsic properties of a PFR there was a risk of cascade inhibition throughout the reactor, hence of washout of some microbial populations. An acidification cascade leads to washout of the methanogenic population. To solve this, a recirculation connected to the inlet was made, which returned part of the digestate coming out of the reactor. Eqs. (1) and (2) represent the generic equation of the first CSTR ($n = 1$) and the other CSTRs ($1 < n \leqslant N$), composing a PFR with a recycle line.

$$\frac{d\varepsilon_{k,1}}{dt} = \frac{q_{in}}{V_{liq}}(\varepsilon_{k,in}-\varepsilon_{k,1}) + \frac{q_{rec}}{V_{liq}}(\varepsilon_{k,N}-\varepsilon_{k,1}) + \sum_{i=1}^{n} \nu_{k,i}\cdot r_{i,1} \quad (1)$$

$$\frac{d\varepsilon_{k,n}}{dt} = \frac{q_{in}}{V_{liq}}(\varepsilon_{k,n-1}-\varepsilon_{k,n}) + \frac{q_{rec}}{V_{liq}}(\varepsilon_{k,n-1}-\varepsilon_{k,n}) + \sum_{i=1}^{n} \nu_{k,i}\cdot r_{i,n} \quad (2)$$

where q_{rec} is the recycle flow, q_{in} is the inlet system flow, V_{liq} is the working volume of each CSTR, $\varepsilon_{k,in}$ is the concentration of the *k-th* state variable in the inlet flow, $\varepsilon_{k,n}$ is the concentration of the *k-th* state variable in the *n-th* CSTR, r_i and $\nu_{k,i}$ are the reaction rate of the *i-th* process that takes place in the *n-th* reactor and the stoichiometric factor for the *k-th* state variable related to that *i-th* process, respectively.

2.3. Non-ideal mixing approaches

2.3.1. Two-region scheme

The first assessed scheme was the TR approach presented by Bello-Mendoza and Sharratt (1998), whose application, together with a kinetic model of the AD process, has already been tested (Keshtkar et al., 2003). This approach considers the imperfect mixing by dividing the CSTR into two perfectly mixed reactors where there is an exchange flow between both reactors (Fig. 1a). Both regions are separated and perfectly mixed with a variable flow transfer. The parameter *a* represents the volume proportion of both regions and *b* the flow exchanged. This approach takes two important assumptions into account: (1) mass transfer between the liquid and gas phase only takes place in the flow region; and (2) the flow exchange between each CSTR connected in series occurs only through the flow region.

With this approach, the total number of equations doubles (except for the gas mass transfer) since each region must be treated as a new digester, so the same mass balance needs to be solved in all the regions. The equations that need to be solved in each region are shown below:

Flow-through region (FR):

$$\frac{d\varepsilon_{k,1,FR}}{dt} = \frac{1}{a_1 * V_{liq}}(q_{in}\cdot\varepsilon_{k,in} + q_{rec}\cdot\varepsilon_{k,N,FR} + q_{1,RR}\cdot\varepsilon_{k,1,RR} - (q_{in} + q_{rec} + q_{1,RR})\cdot \varepsilon_{k,1,FR}) + \sum_{i=1}^{m} \nu_{k,i}\cdot r_{i,1,FR} \quad (3)$$

$$\frac{d\varepsilon_{k,n,FR}}{dt} = \frac{1}{a_n\cdot V_{liq}}((q_{in} + q_{rec})\cdot\varepsilon_{k,n-1,FR} + q_{n,RR}\cdot\varepsilon_{k,n,RR} - (q_{in} + q_{rec} + q_{n,RR})\cdot \varepsilon_{k,n,FR}) + \sum_{i=1}^{m} \nu_{k,i}\cdot r_{i,n,FR} \quad (4)$$

Retention region (RR):

$$\frac{d\varepsilon_{k,n,RR}}{dt} = \frac{1}{(1-a_n)\cdot V_{liq}}(q_{n,RR}\cdot\varepsilon_{k,n,FR} - q_{n,RR}\cdot\varepsilon_{k,n,RR}) + \sum_{i=1}^{m} \nu_{k,i}\cdot r_{i,n,RR} \quad (5)$$

where a_n is the relative volume fraction of the flow region with respect to the total volume for the *n-th* CSTR and $q_{n,RR}$ is the flow between the flow and retention regions for the *n-th* CSTR such that $q_{n,RR} = b_n\cdot q_{in}$. $\varepsilon_{k,n,FR}$ and $\varepsilon_{k,n,RR}$ are the concentrations of the *k-th* state variable in the *n-th* CSTR, for the flow and retention region, respectively. Likewise, $r_{i,n,FR}$ and $r_{i,n,RR}$ are the reaction rates of the *i-th* process that takes place in the *n-th* CSTR, for the flow and retention region, respectively. The