Kinetic modelling of anaerobic digestion with new fractionation using simple model and ADM1

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Abstract
This paper investigates the development of a simple model for the optimization of codigestion not only using the Biochemical Methane Potential (BMP) but also using the degradation kinetics. This study concerns an experimental work on the implementation and the operation of continuous reactors fed with different fruits and vegetables wastes at different organic loading rates. A simple model was developed dividing the substrate into three fractions of rapidly, moderately and slowly biodegradable organic matter using the biogas production curve from batch reactors. This model was applied to experimental data obtained in continuous mode to test its prediction capabilities: a good agreement between experimental and predicted data was found. Furthermore, the monitoring of the evolution of the different fractions of the substrate over time for continuous operation was carried out. The advantage of this simple model is that it allows optimizing the mix of substrates and determining the organic loading rate at which the available substrate is not completely degraded. In addition, the model makes it possible to monitor the dynamical behavior of each fraction.
In parallel, a modified ADM1 model was calibrated using the same data and the same fractionation of the organic matter in three compartments. Satisfying results were obtained, suggesting that the use of the simple model may be useful to identify the different fractions of organic matter and monitor their behavior during co-digestion.

Keywords
Anaerobic digestion; solid waste; fractionation; kinetics; modeling, co-digestion.

INTRODUCTION

The anaerobic digestion is one of the most interesting process for treating various organic wastewater and solid waste, especially agricultural products and agro-industrial wastes, because it combines energy production with organic matter removal (Fezzani et Ben Cheikh., 2008). It is an attractive biotechnological method for reducing the pollution caused by organic wastes (Bouallagui et al., 2004). This process requires specific environmental conditions and different bacterial populations. Mixed bacterial populations degrade organic compounds to produce as end-product a valuable high energy mixture of gases (methane – $CH4$ and carbon dioxide – $CO2$) (Lastella et al., 2002). To formalize available knowledge, to optimize process operation or to monitor anaerobic digesters, several models of AD have been developed (Batstone et al., 2002**)**. In this study, assuming constant kinetics, a simple model was developed, compartmenting the organic matter into three fractions that are the rapidly, moderately and slowly biodegradable material. The model was calibrated using batch experiments and, applied to digesters operated in continuous mode for predicting biogas production, methane yield and the behavior of the three fractions. The results were then compared with simulations obtained with a version of ADM1 which includes the same organic matter fractionation.

MARERIALS & METHODS

Reactor operation

Batch and continuous experiments were carried out in double-walled reactors of 6L effective volume, maintained at 37 °C by a regulated water bath. Mixing in the reactors was done by a system of magnetic stirring. Biogas production was measured on line by Milligascounter MGC-1 flow meters (Ritter gas meters) fitted with a 4-20 mA output**.** The software Odin Silex developed at the INRA laboratory was used to acquire the data. The reactors were seeded at a volatile suspended solids concentration (VSS) of around 15 g VSS/l with anaerobic sludge taken from an industrial-scale anaerobic UASB reactor treating the effluents from a sugar refinery.

In order to assess the kinetic parameters used in modelling, successive batchs were run (6 to 8 batches) with a S_0/X_0 ratio of 0.07 g VS/g VSS. In continuous mode, each reactor was fed with the substrates 5 times per week at different organic loading rates (OLR) of 0.5, 1 and 1.5 g VS/L/day.

RESULTS AND DISCUSSION

A simple model with constant kinetics evaluated in batch mode

In this study, a simple model was developed using data acquired in batch reactors. The first modeling step consisted in classifying the organic matter into three fractions with different degradation kinetics, assuming that the degradation kinetics of each fraction was constant. To do so, it was assumed that the biogas curve was the sum of three kinetics of the three fractions representing the behavior of the rapidly, moderately and slowly biodegradable matter. In Garcia et al., 2015**,** the biodegradable matter was divided into only two fractions (slowly and rapidly biodegradable material). This fractionation has been shown to be appropriate to model bioaccessibility of waste activated sludge (Mottet et al.,2013) and can used to estimate the kinetic coefficients of disintegration and hydrolysis stages of particulates complex substrates(Garcia et al., 2015). However, in our case, two fractions were not enough to obtain satisfying results and instead, three kinetics (and thus three fractions) were used. The substrate concentration was expressed in ml of biogas potentially produced from the degradation of the substrate and not in g/L such as in Durruty et al., 2013.

In practice, six parameters were identified from the batch experiments (The three kinetics and the 3 fractions of the initial substrate) according to the procedure described here after. Substrate concentration at t = 0 was denoted S(0): it represents the maximum amount of biogas to be produced from the degradation of all the substrate introduced. S at time t was calculated by the difference between S(0) and the accumulated biogas produced at time t. The kinetics of degradation of each fraction were supposed to be of zero order and were written as:

Eq (1): $S_1(t) = \max(S_1(0) - k_1 * t, 0)$

Eq (2): $S_2(t) = \max(S_2(0) - k_2 * t, 0)$ ⟶ Eq (4): $S_{Total}(t) = \sum S(t) = S_1(t) + S_2(t) + S_3(t)$

Eq (3): $S_3(t) = \max(S_3(0) - k_3 * t, 0)$

⟶ Eq (5): Gas produced at t = $- S_{Total} + S_1(0) + S_2(0) + S_3(0)$

Where:

- k_1 (ml/h), $S_1(0)$ (ml): parameters of the rapidly biodegradable fraction,
- k_2 (ml/h), $S_2(0)$ (ml): parameters of the moderately biodegradable fraction,
- k_3 (ml/h), $S_3(0)$ (ml): parameters of the slowly biodegradable fraction.

The max operator between $S_i(t)$ and 0 is used to guarantee the positivity of S_i.

Using this simple model, a fractionation of the organic matter of different solid substrates into rapidly, moderately and slowly biodegradable fractions was performed on data acquired in batch reactors using "Matlab" and the 6 unknown parameters were identified using the biogas curve that is to say the respective initial fractions of each "substrates" $S_1(0)$, $S_2(0)$, $S_3(0)$ and the three constant kinetics k_1, k_2, k_3 for rapidly, moderately and slowly biodegradable fractions, respectively.

Experimental validation in continuous operation:
The aim of the work carried out in continuous mode was to validate the use of the kinetic data assessed in batch to model biogas production from digesters operated in continuous. Experimental biogas production from digesters fed with individual substrates at different OLRs was compared with the biogas production foreseen by the model. The experiments were carried out with three fruits and vegetable (carrot, banana, potato) which were individually used to feed reactors operated in continuous mode at different OLRs (0.5, 1 and 1.5 g VS/L/d). An example with carrot at an OLR of 0.5 g VS/l/d is given in figures 1 and 2. In Figure 1, the comparison between the prediction of cumulated biogas production using the simple model (identified using data obtained from batch experiments) and experimental data obtained from continuous experiments is shown at an OLR of 0.5 g VS/L/d. The correspondence between the experimental biogas production and that given by the model was excellent. In Figure 2, the simulation of the evolution with time of the different fractions is shown. This figure shows that at an OLR of 0.5 g VS/L/d, all the organic fractions contained in the carrot were degraded. This was confirmed by the methane yield obtained in continuous operation (338 ml CH_4/g VS) which was close to the average value obtained previously during experiments performed in batch mode (326 ml CH_4/g VS), with a different batch of substrate.

The same experiments were simulated using an ADM1 model calibrated for solid wastes. A good correlation was found (see Figure 3) and the simulations were almost the same than those obtained with the simple model which validates the hypothesis of the proposed fractionation of the substrate in three compartments.

In perspectives, the model will be further validated using different residues in codigestion (two substrates and more) at different OLRs. The aim is to develop and validate a simple co-digestion model which can be used mainly for substrate management during the design of co-digesters (Optimization of the mixes of substrates using degradation kinetics and not only BMPs) and during the operation of co-digesters at industrial scale (effect of the addition of a new substrate, optimal conditions for the addition of a new substrate, …).

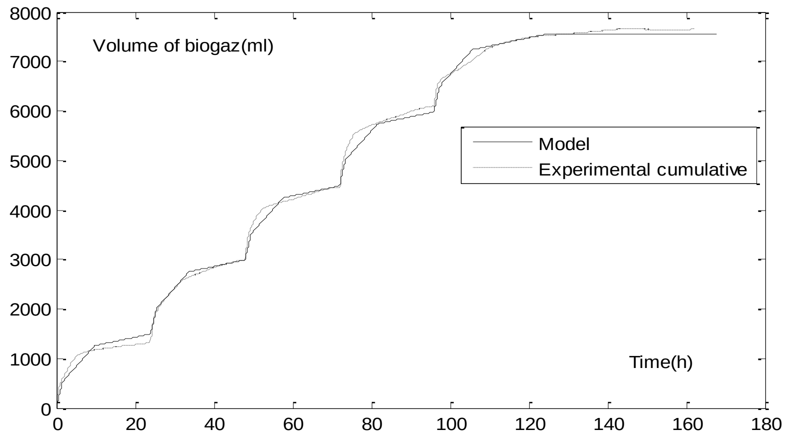

Figure 1. Comparison of the experimental and modeled biogas production for carrot at an OLR of 0.5g VS/l/d.

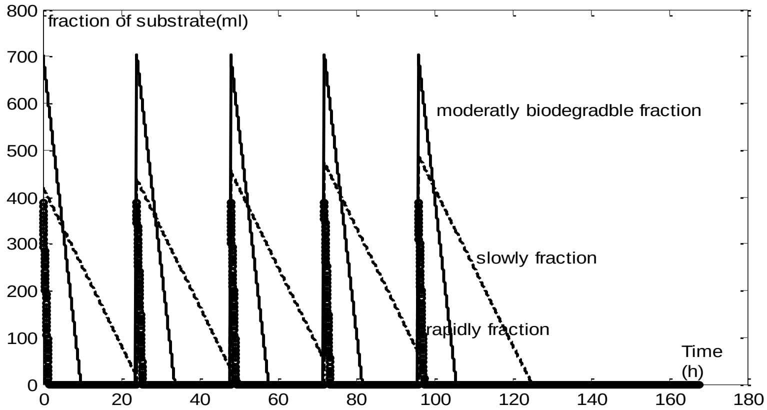

Figure 2. Evolution during one week of the three biodegradable fractions for carrot at an OLR of 0.5 g VS/L/d.

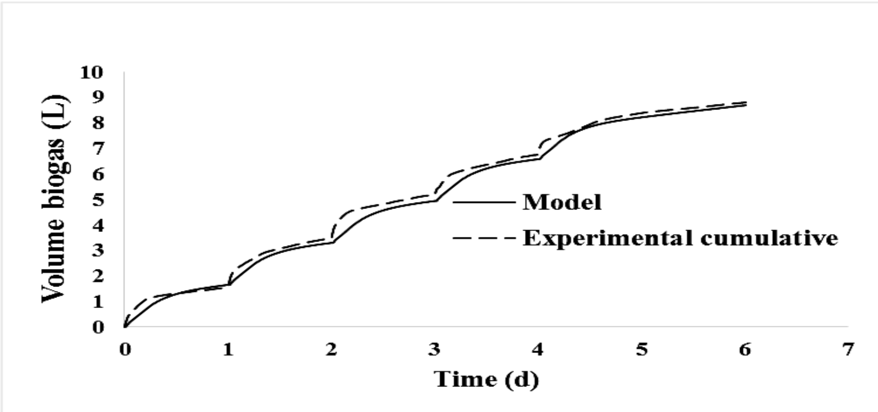

Figure 3. Modelling with modified ADM1 model for carrot at an OLR of 0.5 g VS/L/d.

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