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Modelling the anaerobic digestion of solid organic waste – Substrate characterisation method for ADM1 using a combined biochemical and kinetic parameter estimation approach

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ABSTRACT

This work proposes a novel and rigorous substrate characterisation methodology to be used with ADM1 to simulate the anaerobic digestion of solid organic waste. The proposed method uses data from both direct substrate analysis and the methane production from laboratory scale anaerobic digestion experiments and involves assessment of four substrate fractionation models. The models partition the organic matter into a mixture of particulate and soluble fractions with the decision on the most suitable model being made on quality of fit between experimental and simulated data and the uncertainty of the calibrated parameters. The method was tested using samples of domestic green and food waste and using experimental data from both short batch tests and longer semi-continuous trials. The results showed that in general an increased fractionation model complexity led to better fit but with increased uncertainty. When using batch test data the most suitable model for green waste included one particulate and one soluble fraction, whereas for food waste two particulate fractions were needed. With richer semi-continuous datasets, the parameter estimation resulted in less uncertainty therefore allowing the description of the substrate with a more complex model. The resulting substrate characterisations and fractionation models obtained from batch test data, for both waste samples, were used to validate the method using semi-continuous experimental data and showed good prediction of methane production, biogas composition, total and volatile solids, ammonia and alkalinity.

1. Introduction

The Anaerobic Digestion Model 1 (ADM1) (Batstone et al., 2002) is to date the most comprehensive and widely used model of the anaerobic digestion (AD) process, and describes the main biochemical reactions and physico-chemical processes in anaerobic digestion. Substrate characterisation is ultimately the most influential model input on methane flow prediction (Solon et al., 2015) and a recent review identified that the development of feedstock characterisation methods to provide the required model inputs was still a bottleneck to a broader adoption of ADM1, with more work required in this topic (Batstone et al., 2015).

For each substrate ADM1 requires a physico-chemical characterisation, in terms of its biochemical make-up (carbohydrate, proteins, lipids) and charge bearing compounds (acids, bases, salts). The kinetic characteristics of the substrate (inert content and rapidity of degradation) are also needed as inputs. As well as determining the kinetics of biogas production the substrate characteristics further influence ADM1 predictions in the following ways (Batstone, 2013):

- Gas composition is inherently dependent on the input carbon oxidation state.
- Complex substrates are composed of different fractions which degrade at different rates.
- Buffering compounds (e.g. carbonate and ammonium salts) available in the substrate contribute to the physico-chemical system (e.g. pH) and therefore to many biological inhibition effects.

Two main methods have been implemented for the physico-chemical characterisation: Either from direct analysis of the biochemical fractions (Astals et al., 2013; Koch et al., 2010) or from elemental analysis (Kleerebezem and Van Loosdrecht, 2006; Zaher et al., 2009). However the parameters describing the kinetics of

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Nomenclature

Where possible we have maintained the nomenclature used in ADM1 in order to facilitate understanding and the reader can refer to both the original ADM1 description (Batstone et al., 2002) for a comprehensive description.

Symbol	Meaning
C_i	carbon content of biochemical fraction (i) in ADM1
f_{ch}	carbohydrate/sugar fraction of substrate
f_d	degradable fraction of substrate
f_{li}	lipid/fatty acid fraction of f_d
f_{pr}	protein/amino acid fraction of f_d
f_s	soluble fraction of f_d
k_{hyd}	hydrolysis constant for particulate fraction
$k_{hyd,r}$	k_{hyd} for rapidly degradable particulate fraction
$k_{hyd,s}$	k_{hyd} for slowly degradable particulate fraction
N_i	nitrogen content of biochemical fraction (i) in ADM1
P_{ka}	acid dissociation constant
P_{kw}	dissociation constant for water
r^2	coefficient of determination
S	soluble substrate concentration
X	particulate substrate concentration
$\overline{y_m}$	average measured methane production
$y_{m,i}$	measured methane production
$y_i(p)$	modelled methane production
α	charge per unit COD for ionic balance
ρ_s	density of substrate
$\sigma_{m,I}$	standard error of measurement

Subscripts

aa	amino acid
ac	acetic acid
an	anion
bu	butyric acid
c	composite organic matter (from biomass decay)
cat	cation
ch	carbohydrate
fa	long chain fatty acids
hyd	hydrolysis
I	inert (non-biodegradable)
IC	inorganic carbon
IN	inorganic nitrogen
li	lipids
pr	protein
pro	propionic acid
s	slowly degradable fraction
su	sugar
r	readily degradable fraction
va	valeric acid

degradation have been usually determined through calibration or parameter estimation (Lübken et al., 2007; Thamsiriroj and Murphy, 2011; Wichern et al., 2009) byt comparing model outputs with experimental data. It has been found, when complex particulate substrates are modelled, that the substrate is best described as composed of several fractions with different degradation rates. In these cases the default formulation of ADM1 needs to be updated to include these new state variables. This has been the approach of some studies (Mottet et al., 2013; Yasui et al., 2008), and in particular the work of Girault et al. (2012) and García-Gen et al. (2015) who developed methods based on batch tests to determine the kinetic fractionation. However both of these methods rely on a visual interpretation of experimental methane production data and therefore introduce some subjectivity to the obtained model parameters.

This paper proposes an improved methodology for substrate characterisation for use with ADM1 involving a combined biochemical and kinetic approach, i.e. based on elemental analysis of the sample and data from bioreactor experiments. Four substrate fractionation models are integrated into ADM1 and evaluated for their ability to describe the anaerobic digestion of source segregated food waste (FW) and green wastes (GW). We aim to remove the subjectivity of existing kinetic fractionation methods by comparing the alternative fraction models using both quality of fit and uncertainty in the calibrated parameters. Furthermore the described methodology, based on data from batch testing, is evaluated and validated using data from semi-continuous the experiments. The proposed methodology is intended to be used to estimate the characteristics of any given substrate to predict the performance of anaerobic processes, including co-digestion.

2. Materials and methods

2.1. Experimental methods

2.1.1. Materials

Household segregated FW and GW were collected at a local recycle centre and stored at 5 °C. Within 24 h, the substrates were examined and large pieces of bone, plastic, metal, wood were removed to avoid damage to the homogenisation equipment and reduce sampling errors during later analysis. The substrates were then homogenised using a mincer to an average particle size of 1 mm, sampled for chemical analysis, and the remaining part was stored at −18 °C and thawed before feeding to the digesters.

2.1.2. Batch tests

Batch tests were carried out in 500 ml laboratory digesters, in triplicate for both substrate and blank (inoculum only), with a working volume of 350 ml. The temperature of the digestion was maintained at 37 °C, to mimic the temperature of a conventional mesophilic AD system, by immersion in a water bath. Agitation was supplied by a vertical stirrer operated at 60 RPM as per the default setting of the equipment manufacturer (Bioprocess Control). The inoculum was obtained from a mesophilic digester treating primary sludge at a wastewater treatment plant. It was screened through a 0.5 mm sieve and then incubated for 4 days in the bottles to allow the degradation of most of the residual easily degradable matter. Before feeding the substrate, the inoculum was sampled for analysis.

The mass of substrate added was calculated on the basis of a defined chemical oxygen demand (COD) based substrate to inoculum ratio (2.5 $gVS_{inoculum}/gCOD_{substrate}$). Thisratio reduces inhibition effects and accumulation of intermediary compounds during substrate degradation (Raposo et al., 2012), therefore allowing hydrolysis rate limiting conditions for methane production from the particulate fractions. After adding the substrate in the digesters, the headspace was purged with pure nitrogen. The produced gas was scrubbed into a 3 M NaOH alkaline solution in order to remove the carbon dioxide and the hydrogen sulphide. The volume of scrubbed gas was then measured through an AMPTSII system (Bioprocess Control), with a resolution of 10 mL. Methane production is reported at STP (0 C and 1 bar) and calculated assuming a scrubber efficiency of 98%, subtracting the concentration of water vapour, and taking into account the overestimation caused from the initial nitrogen content in the headspace, as detailed in

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