



Early prediction of Biochemical Methane Potential through statistical and kinetic modelling of initial gas production



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HIGHLIGHTS

- BMP can be predicted at a much earlier stage into a test.
- BMP data from 138 samples divided into five groups are presented.
- 61 different prediction algorithms are evaluated for best performance.
- Linear regression of previous test results are important for accurate predictions.

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ABSTRACT

A major drawback of Biochemical Methane Potential (BMP) tests is their long test duration, which could be reduced substantially if the final gas production could be predicted at an earlier stage. For this purpose, this study evaluates 61 different algorithms for their capability to predict the final BMP and required degradation time based on data from 138 BMP tests of various substrate types. By combining the best algorithms it was possible to predict the BMP with a relative root mean squared error (rRMSE) of less than 10% just 6 days after initiation of the experiment. The results from this study indicate that there is a possibility to shorten the test length substantially by combining laboratory tests and intelligent prediction algorithms. Shorter test duration may widen the possible applications for BMP tests in full-scale biogas plants, allowing for a better selection and proper pricing of biomass.

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1. Introduction

With an increasing demand for efficient waste handling and fossil fuel replacement, anaerobic digestion has gained a lot of attention in the recent time. In Europe, the biogas production has increased substantially in the last few years with a rise from 3.8 Mtoe in 2003 to 12.0 Mtoe in 2012 (EurObserv'ER, 2005, 2013). The growing interest for production of biogas by anaerobic digestion has led to an increased demand for finding and evaluating new types of suitable feedstock.

A method to source and determine the feasibility of a material to serve as a substrate in anaerobic digestion is represented by the Biochemical Methane Potential (BMP) test. Such a test monitors the gas production following the incubation of an organic material with an anaerobic bacteria mixture under well-controlled

conditions (Angelidaki et al., 2009). The BMP test provides information on the extent of the process and decomposition rate of a material for biogas production, which are valuable parameters in the design and operation of a biogas plant (Chynoweth et al., 1993; Lesteur et al., 2010; Moody et al., 2009; Raposo et al., 2011).

One major drawback with conventional BMP tests is their long duration. Often 30–60 and sometimes up to 100 days are necessary to obtain the required results, which means that there is an extensive delay before actions can be taken (Lesteur et al., 2011; Ponsá et al., 2011). Consequently, the tests are mainly used for pre-studies, mandatory degradation tests or various scientific applications. However, if results could be obtained faster, BMP tests would likely be of interest for industrial biogas producers as well, as this would allow them to use the test for quality checks and pricing of substrates.

Previously suggested approaches to obtain quick BMP results are the use of empirical relationships based on the material's chemical and biochemical composition (Thomsen et al., 2014) or respirometric activity (Scaglia et al., 2010) as well as methods

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using Near-Infrared Spectroscopy (NIRS) (Doublet et al., 2013). A more general overview of each technique can be found in the review article by Lesteur et al. (2010). These approaches show great potential as they allow immediate results within reasonable error margins. However, as their predictions are based on time independent measurements, these techniques do not offer any information regarding the kinetic degradation of the material. Moreover, the absence of a biological anaerobic degradation process, limits the information about the toxicity and loading rate of the substrate.

An alternative method to obtain quick BMP results, with the kinetic and biological degradability information included, is the combination of conventional BMP tests and numerical prediction models. Promising results in this regard have been achieved by Ponsá et al. (2011), observing strong linear correlations between the biogas production at different times in a test and the final value for different types of organic fraction of municipal solid wastes (OFMSW). This suggests that, given a big enough database, it is possible to statistically predict the final BMP of a sample.

It is commonly known that well-controlled batch degradations follow certain kinetic patterns that can be modelled using suitable kinetic models. For complex materials, limited by hydrolytic degradation of particulate matter, a first order rate equation is generally used to describe the degradation profile (Shahriari et al., 2012). Several other model types have also been proposed as more accurate alternatives for different types of substrates (Beuvink and Kogut, 1993; Koch and Drewes, 2014; Rincón et al., 2010). This suggests that, given a reliable set of initial data and an accurate kinetic model, it is possible to predict the remaining methane potential for many different types of materials. As this approach includes the biochemical aspects of anaerobic digestion, key information about the material's toxicity and loading strain on the microbial population is also obtained. The recent development of specialised laboratory equipment, such as Automatic Methane Potential Test System (AMPTS) II, which allows automatic and reliable gas measurements with high resolution, makes an approach based on real-time prediction with mathematical models highly feasible.

The current study evaluates 61 different algorithms for their ability to predict the BMP of various substrate types. Special emphasis is directed towards finding the most suitable model and the time required to produce estimations within an acceptable error range.

2. Methods

2.1. Equipment

The Automatic Methane Potential Test System II (AMPTS II, Bioprocess Control Sweden AB) was used for the BMP analysis of the target substrates. The AMPTS II is a standardised laboratory set-up specially designed for automatic BMP determination of any biodegradable material. The gas is measured through water displacement using pre-calibrated flow cells that give a signal for each 10 mL of produced gas. Temperature and pressure sensors are used to normalise the gas volume to 0 °C, 1 atm and dry gas conditions at each measurement point.

2.2. Materials

The BMP was investigated for 138 individual samples divided into six different groups. In order to describe the experimental variation in a BMP test each replicate (in most cases triplicates) of a sample was included in the study, making a total of 380 investigated datasets. The studied sample groups were *anaerobic sludge* (i.e. effluent from anaerobic digesters), *standard compounds* (e.g.

cellulose, starch, gelatine), *household waste* (e.g. fruit and vegetable waste, milk waste, meat waste, co-digestion mixtures), *agricultural waste* (e.g. wheat straw, bamboo waste, banana stem), *sewage sludge* (e.g. primary and secondary sludge, co-digestion mixtures) and *lipid rich waste* (e.g. butter waste, oil waste). The majority of the BMP tests were performed using inoculum collected from a sewage treatment plant (Ellinge sewage plant, Sweden), which receives municipal wastewater and vegetable residues from the food industry and operates at mesophilic temperatures.

Sodium hydroxide (reagent grade 97%, Sigma–Aldrich) and thymolphthalein pH indicator (dye content 95%, Sigma–Aldrich) were used for the preparation of 3 M alkaline solution for CO₂ fixation. N₂ gas (Air Liquid Gas AB, Sweden) was used to obtain anaerobic conditions during the sample preparation phase.

2.3. Experimental procedure

The biodegradability of the samples was determined using BMP assays as described in Strömberg et al. (2014b). The majority of the tests were performed at 37 °C with an inoculum to substrate ratio of 2 based on volatile solids (VS) amount. An active volume of 400 ml in 500 ml bottles was used in all tests and mixing was performed mechanically, either intermittently or continuously. Blanks containing only inoculum were included in every test and used to deduct the background gas production from the inoculum. No external nutrients or trace elements were added to the reactors before starting the BMP tests. All data was sampled with 10 mL resolution and converted to hourly basis (i.e. one data point per hour). The BMP (adjusted to 0 °C, 1 atm and dry condition) was calculated by subtracting the gas production of the inoculum from the gas production of the sample and dividing it by the amount of VS added.

2.4. Numerical and statistical details

2.4.1. Data structure

In total 380 sample datasets from 138 individual samples, spread over six groups, were included in the study. The samples in each sample group were further randomly divided into a calibration and a validation set containing 67% and 33% of the samples, respectively. This procedure was repeated five times so that the samples were represented in both the calibration and validation set several times. All results presented in this study are based on the average of these five validation sets.

2.4.2. Statistical parameters

Three statistical parameters (i.e. relative root mean squared error of prediction (rRMSE), relative absolute error (rAE) and the coefficient of determination (R^2)) were calculated according to Eqs. (1)–(3):

$$\text{rRMSE} = \frac{\sqrt{\sum (y_i - \hat{y}_i)^2}}{\bar{y}} \quad (1)$$

$$\text{rAE} = \frac{\sum \left(\frac{|y_i - \hat{y}_i|}{y_i} \right)}{n} \quad (2)$$

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (3)$$

In Eqs. (1)–(3), y_i and $\hat{y}_i$ are the experimental and predicted values, respectively, for sample i , n is the number of samples and $\bar{y}$ is the mean of the experimental values.

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