Anaerobic Digestion Model based on Mass Balances. Development, Implementation and Validation.

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Abstract
The paper presents a new mathematical model of anaerobic digestion based on mass balances of organic dry matter (oDM) and nitrogen. The model was used for simulation of two agriculture biogas plants. The results of simulation in respect of biogas and methane yield, concentrations of ammonium nitrogen and dry matter (DM) in digested sludge, showed a satisfying compliance with measurements. Based on the results of validation further application of the model, as for example real-time simulator for control of anaerobic digestion process on the biogas plants, is promising.

Keywords
Anaerobic digestion, mathematical modelling, renewable energy, control of biogas plants

INTRODUCTION

Meanwhile, there are several mathematical models that describe the anaerobic degradation (Gavala *et al*. 2003, Prause *et al.* 1997). The IWA Task Group on Mathematical Modelling of Anaerobic Digestion Process has developed the Anaerobic Digestion Model No. 1 (ADM1) (Batstone *et al.* 2002). This most popular model is based on the balance of chemical oxygen demand (COD). Numerous simulation studies were performed with the use of this model for biogas plants (Cimatoribus 2009, Wichern *et al.* 2008, Wolf *et al.* 2007). Although good adjustments with the real results have been achieved, the calibration and use of the model is restricted due to its complexity.

Using the currently available measurement the determination of a number of important control parameters for anaerobic digestion such as: the degradation rate of the substrate, the specific methane and biogas yield, the buffer capacity, concentrations of organic acids and ammonium nitrogen is no possible or often only with great effort (Kujawski *et al.* 2009). Those parameters can be estimated through real-time simulation (during the operation of the plant). For various reasons, the use of currently available mathematical models of anaerobic digestion processes (such as ADM 1) for the real-time simulation, and for the control and regulation of the biogas plants is difficult. Therefore a new a new approach was developed.

MATERIALS AND METHODS

Basics of the developed model

The model is based on mass balances of organic dry matter and nitrogen as well as on the simplified description of the kinetics of anaerobic degradation and ammonium production. Because of the very long hydraulic retention time of the substrates in the system (60-100 days), the digester, which is originally continuously fed, is implemented in the model as a continuous stirred tank reactor (CSTR). The model was implemented using MATLAB®.

In contrast to complex models the degradation of the dosaged portion of specific substrate the biomass is described with the following balance equation:

$$V \cdot \frac{dc_{oDM,\deg}}{dt} = Q_I \cdot c_{oDM,\deg,I} - Q_E \cdot c_{oDM,\deg} - c_{oDM,\deg} \cdot V \cdot f_d(t) \qquad \textbf{Equation 1}$$

where: $c_{oDM,\deg}$ - concentration of degradable oDM [kg/m^3], $c_{oDM,\deg,I}$ - concentration of degradable oDM in the influent to the digester [kg/m^3], Q_I - influent to the digester [m^3/d], Q_E - effluent from the digester [m^3/d], $f_d(t)$ - total kinetic rate of digestion [1/d], t - time [d], V - active volume of the digester [m^3]

The total kinetic rate of the anaerobic digestion of organic dry matter for specific substrate is derived directly from the empirically determined batch biogas yield measurement $f_g(t)$ (equation 2).

$$f_d(t_i) = \frac{df_g(t_i)}{dt} \cdot \frac{1}{f_g(t_\infty) - f_g(t_i)} \quad \textbf{Equation 2;} \qquad Q_B = \gamma \cdot c_{oDM,\deg} \cdot V \cdot f_a(t) \left[\frac{m^3}{h} \right] \quad \textbf{Equation 3}$$

Where: γ - biogas production in unit per mass of degradable organic dry matter [m^3/kg]

In the frame of this work no batch biogas yield measurements were performed, so the curves were obtained on base of the literature and digitized. Biogas production (Q_B) is calculated using the equation 3. Biogas production per unit mass of degradable organic dry matter was calculated using equation 4.

$$\gamma \approx \frac{22{,}413 \frac{m^3}{kmol}}{v_{CH_4} \cdot 16 \frac{kg}{kmol} + v_{CO_2} \cdot 44 \frac{kg}{kmol}} \quad \textbf{Equation 4;} \qquad Q_{CH_4} = Q_B \cdot v_{CH_4} \quad \textbf{Equation 5}$$

Where: v_{CH_4} - concentration of methane in the biogas [%], v_{CO_2} - concentration of the carbon dioxide in the biogas [%]

For the calculation of the methane production it was assumed that the produced biogas from a definite substrate has constant methane content. Hence the production of methane Q_{CH_4} is calculated using the equation 5

The calculation of the ammonium nitrogen concentration requires usually accurate accounting on all nitrogen fractions and the nitrogen cycle. Even for detailed models of anaerobic digestion, such as ADM 1, this task is difficult due to the complexity of the anaerobic processes. In this model the concentration of the ammonium nitrogen was calculated using the assumption that nitrogen is distributed homogeneously in the degradable organic solids. The concentration of ammonium nitrogen in the reactor was calculated using the following equation:

$$V \cdot \frac{dc_{NH_4-N}}{dt} = Q_I \cdot c_{NH_4-N,I} - Q_E \cdot c_{NH_4-N} + V \cdot f_{NH_4-N}(t) \cdot c_{N,\deg} \quad \textbf{Equation 6}$$

where: $c_{N,\deg}$ - concentration of particulate degradable nitrogen in the degradable oDM [kg/m^3], $c_{NH_4-N,I}$ - concentration of ammonium nitrogen in the influent of digester [kg/m^3], $f_{NH_4-N}(t)$ - total kinetic rate of the release of ammonium nitrogen [1/d]

In the frame of this work no studies for investigation of the total kinetic rate of ammonium release were made. It was assumed that this parameter is equal to the total kinetic rate of the anaerobic degradation $f_d(t)$.

Details of investigated biogas plants

The investigated agricultural biogas plants *Lelbach* and *Wambeln* for which the model was validated are described in Kujawski *et al.* (2009).

RESULTS AND DISCUSION

In the first months of operation of the biogas plant *Lelbach* the amount of biogas estimated by the help of the model was higher than measured biogas production (Figure 1a). Reasons for that could be slower development of a stable the biocoenosis or high concentrations of organic acids in the delivered for setup inoculum. From day 180 the results show a good accordance between the simulated and the measured data. It is evident that the dynamics of the processes is well reproduced.

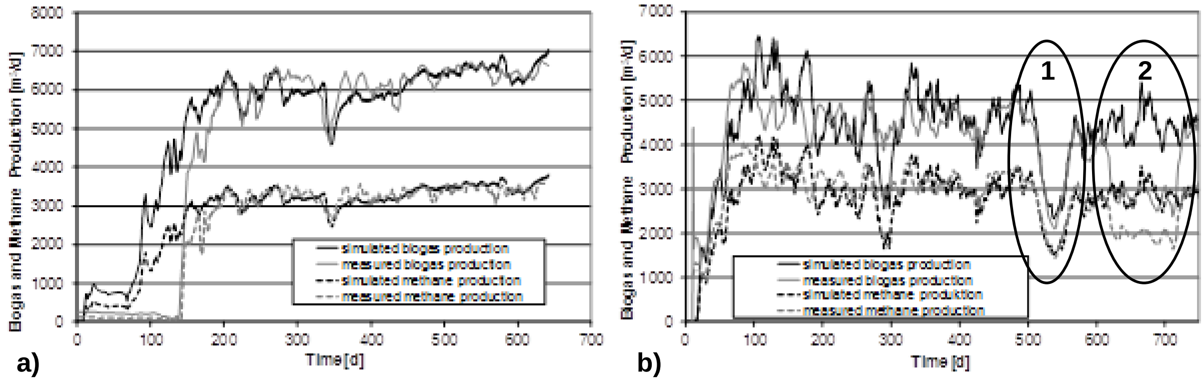


Figure 1. Measured and simulated methane and biogas production, a) biogas plant *Lelbach*, b) biogas plant *Wambeln*

Figure 1b shows the results of the simulation and measured data for biogas plant *Wambeln*. In the period in which the substrate supply has been strongly reduced (marked as "1" in Figure 1b) it is obvious that the simulated and measured biogas production are in compliance. In this period numerous substrate investigations for DM and COD contents were carried out. As "2" (Figure 1b) the period has been marked in which the simulated biogas production was significantly higher than the measured production of biogas. During this period a high amount of produced biogas was lost due to a large leak in the gas storage membrane.

It can be seen that in both plants the simulated methane and biogas production correspond well temporarily with the measured values. Reasons are that the DM and oDM measurements were performed only for a few substrates and samples and total kinetic rates for digestion of substrates were assumed on the base of batch biogas yield measurements from literature.

Figure 2a shows the results of the simulation an measurements of the NH_4-N concentration in the primary and secondary digester of the biogas plant *Lelbach*. It can be seen that the NH_4-N concentration in the primary digester is higher than in the secondary digester. This is because a main part of the substrates was supplied directly to the primary digester. Thus, during the degradation of organic matter, nitrogen was released as ammonium nitrogen. Nevertheless, it is apparent that the difference between the measured values in the first and second digester was reproduced well in the simulation.

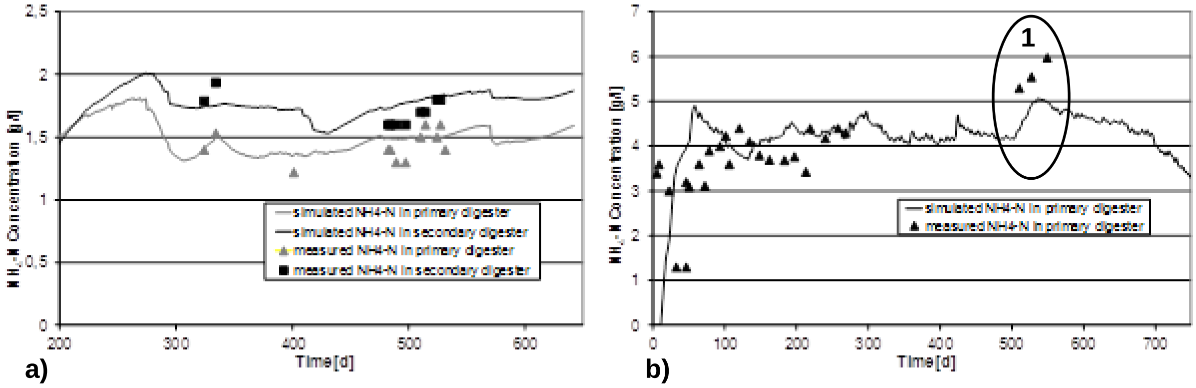
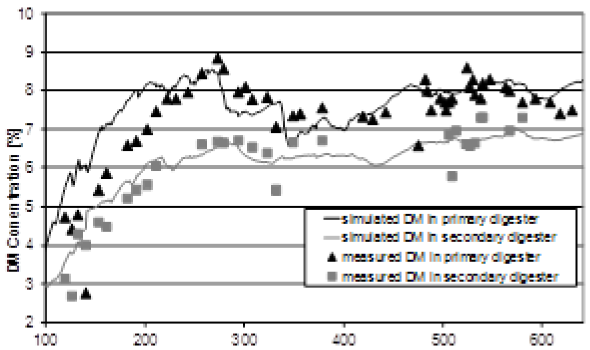


Figure 2. Measured and simulated NH_4-N concentrations for the digesters, a) biogas plant *Lelbach*, b) biogas plant *Wambeln*

The simulation results for the BGA *Wambeln* can be found in Figure 2b. Unfortunately only a few measurements of the NH_4-N in the sludge and the N_{tot} of the substrates were made during the period of this study. Accordingly, these missing values in substrates were assumed for the simulation mainly on base of literature. In the course of further operation the measured ammonium-nitrogen concentrations have increased (Figure 2b, area "1"). For this period values determined by the simulation are lower than those measured on the plant. Nevertheless, the increasing tendency can be seen in the measured values as well as in the simulated curve.

The real plant data and results of DM simulation for the biogas plant *Lelbach* are shown in Figure 3a. Overall, the concentration in the secondary digester was significantly lower. The reason for this difference is subsequent degradation in secondary digester of oDM in digested sludge. Trends and values are produced in proper way through the model.

Although there were only few investigations of the substrates on the biogas plant *Wambeln* the accordance of the simulation results and measurements for DM in the first digester are in good compliance (Figure 3b).



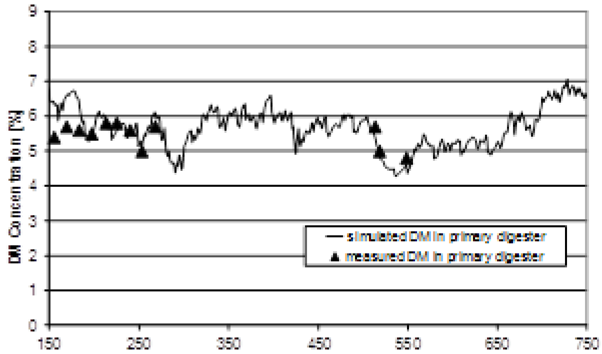


Figure 3. Measured and simulated DM concentrations for the digesters, a) biogas plant *Lelbach*, b) biogas plant *Wambeln*

CONCLUSIONS

A new model for anaerobic digestion, based on mass balances of dry matter and nitrogen, includes two significant innovations: On the one hand the simplified description of the kinetics of anaerobic degradation and production of ammonium and on the other hand, the model is simplified regarding the evaluation of model parameters in comparison with complex models.

The results of validation of the model for two agricultural biogas plants show that NH_4-N, DM, biogas and methane production, were in good accordance with the real data, especially in periods in which the composition of the substrates (feed) was determined. Thereby this model is well suited for real-time simulations (support for the control and regulation) as well as for design of new plants. Nevertheless a minimum of analysis regarding DM and nitrogen contents in the influent of digesters has to be conducted in order to improve the quality of the models output.

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