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ADM1-based modeling of anaerobic codigestion of maize silage and cattle manure – calibration of parameters and model verification (part II)

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Abstract: The aim of this study was to implement ADM1xp model to simulate behavior of anaerobic co-digestion of maize silage and cattle manure. The accuracy of ADM1xp has been assessed against experimental data of anaerobic digestion, performed at OLR = 2.1 gVS $dm^{-3} \cdot d^{-1}$ and HRT = 45d. Due to the high number of parameters in ADM1xp, it was necessary to develop a customized procedure limiting the range of parameters to be estimated. The best fitting of experimental to simulated data was obtained after verification of 9 among 105 stoichiometric and kinetic parameters. The values of objective function (J_C) ranged between 0.003 (for valerate) and 211 (for biogas production).

Introduction

Anaerobic degradation of organic matter is a complex and multi-step process with reactions in which several key groups of bacteria participate. For this reason mathematical modeling using Anaerobic Digestion Model No. 1 (ADM1) is the subject of much research. Up to now, the ADM1 has been tested for municipal wastewater sludge, municipal solid waste, agriculture waste and crop residues. Predicting the performance of anaerobic digestion for agricultural waste mixed with co-substrates at different ratios is important for proper process design and maintenance of stability.

The ADM1 is a structured model, where physical, chemical, and biological processes are included in a biochemical kinetic matrix. The following processes are comprised of disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis. In total, 19 processes, 33 state variables, and 105 stoichiometric and kinetic parameters are involved (Batstone et al. 2002).

This study presents the principles of ADM1xp calibration. The kinetic parameters for reactions of disintegration, aceto- and methanogenesis processes during anaerobic digestion of maize silage and cattle manure mixture are verified. After verification, simulation results are evaluated using a fitness function (J_c) for selected parameters obtained experimentally, i.e. biogas/methane production, pH and volatile fatty acids concentration (acetate, propionate and valerate).

Theoretical background – parameter estimation in ADM1 model

Mathematical models used in biotechnology are comprised of many uncertain parameters (they cannot be easily estimated through direct and indirect measurements) and relatively few measured outputs. This makes the models difficult to calibrate.

Usually, the parameters' values in the ADM1 are derived from a variety of sources, including the results from stirred-tank reactors (STRs) or batch and semi-batch mixed reactors (Batstone et al. 2000, Batstone et al. 2002, Costello et al. 1989, Ramsay 1997, Romli 1993, Siegrist et al. 2002). Some parameters are determined a priori, based on the literature (Batstone et al. 2000, Costello et al. 1989, Ramsay 1997, Romli 1993). Stoichiometric coefficients in the rate equation matrix are taken without any changes, as in the original model (Batstone et al. 2002). In the present study, carbon and nitrogen balance of the feedstock was calculated.

Model calibration must include two objectives: quality of data fitting and estimated parameter confidence. Obtaining a good agreement between the model predictions and the experimental data is always favored by increasing the number of degrees of freedom. For the ADM1, estimation of all parameters would require a significantly broader pool of experimental results (Kesavan and Law 2005). To avoid inappropriate estimation, reduction of the number of parameters is recommended. The parameters requiring adjustment are:

disintegration constants/hydrolysis rates, the half saturation constants for acids ($K_{s,i}$) and the maximum specific uptake rates for acids ($k_{m,i}$). The other parameters can be adopted from Batstone et al. (2002).

The procedure of estimating a minimal number of a subset of parameters, providing the best fitting of experimental to simulated data, is a multi-stage process.

To find a parameter set with the best fitting, the possible equifinality of models should be considered. Equifinality means that there is no simple of optimal parameter set representing a system, but rather several combinations of parameter values for a chosen model structure. For instance, Ge et al. (2010) and Batstone and Keller (2001) specified a parameter by confidence regions, not using single values. The results of several combinations led to the creation of a kind of map, consisting of global and local minima and maxima. By equifinality, the number of modified parameters was reduced to only a few of the most sensitive.

To assess the best fitting of the model to experimental data, several methods can be adopted. The weighted sum of squared errors between model predictions and collected data can be minimized by changing the model parameters (θ). The quality of the model calibration can be evaluated by analyzing the parameter estimation covariance matrix $C(\theta)$. This matrix is calculated by many minimization programs using different techniques (Dochain and Vanrolleghem 2001). The diagonal elements are the variances of the parameter estimates, while the off-diagonal elements are the covariances between different parameters. The covariance matrix can then be used to calculate confidence intervals, confidence regions and parameter correlations. Small variances will result in small confidence regions and more accurate parameter estimations. Wichern et al. (2009) used a genetic algorithm and defined a fitness function as an assessment tool by minimizing the sum of squared differences between the logarithm of measurements and the logarithm of simulated results. Koch et al. (2010) evaluated the agreement between simulated and experimental data using a modified Nash–Sutcliffe coefficient.

In many papers, the coefficients of model fitting to experimental data are used in analysis of model sensitivity. For that purpose, Kim et al. (2006) used a single step variation method (SVM) to identify the sensitivity of a model for digestion of grass. Wichern et al. (2009) determined the sensitivity index from a procedure in which each parameter was changed several times in increments of 10% above and below the nominal value. In the present study, the genetic algorithm optimization procedure, *ga*, was used to determine model coefficients.

Materials and methods

Experiments

Laboratory fermenter

In order to calibrate the ADM1xp, data from laboratory-scale experiments were collected. Anaerobic digestion was performed in a stainless-steel, anaerobic CSTR with a working volume of 100 dm^3 (total volume 120 dm^3). The reactor was equipped with a stirrer with adjustable rotation speed (76 rpm $min.^{-1}$) and a water jacket. The fermentor was semi-continuously fed each day. The volume of added feedstock was the same as the digestate withdrawn. The biogas was collected in Tedlar sample bags each day for 1 h and its composition was measured using a GA 2000+ automatic analyser (Geotechnic Instruments, UK).

Feedstock preparation and experiment set-up

In the experiment, maize silage and cattle manure were used as substrates. These were from a farm in Komorowo (Kujawsko-Pomorskie Region of Poland). The feedstock was composed of maize silage and cattle manure mixed at a ratio of 49:51 (% VS) and diluted with water to obtain a desired concentration of total solids in the influent. The feedstock was prepared by weighting 220 g of maize silage and 641 g of cattle manure. The mixture was diluted with 1361 g of water to obtain 113.5 g kg^{-1} TS and 93.5 g kg^{-1} VS.

Input calculations

The input before running the simulations included the following operational conditions: feeding time and volume, temperature of the reactor and the properties of the feedstock. The fermenter was supplied daily with 2.22 dm^3 of the prepared feedstock. The HRT was 45d and the OLR was 2.1 gVS $dm^{-3} \cdot d^{-1}$. Temperature in the fermenter was maintaining at 39°C by water jacket.

The characterization of the feedstock was based on chemical oxygen demand (COD), concerned particulate, soluble degradable and inert organic matter. A detailed methodology for calculations of values for the influent variables was given in Part I. Some missing values were taken from Batstone et al. (2002) and Rosén and Jeppsson (2006). The values of influent variables are given in Table 5 (Part I). The initial values of stoichiometric coefficients and kinetic parameters used for the simulation were derived from Batstone et al. (2002).

Mathematical model

In the present study, the ADM1xp is a modified version of ADM1. The modification concerns incorporation of the X_p value (concentration of particulate products arising from biomass decay (IFAK 2009). This was proposed by Wett et al. (2006) and implemented by ifak system (Germany).

The modified model is in the form of a differential (25) and algebraic (34) equation system with 33 steady-state variables (substrates, reaction intermediates and gaseous products, i.e. methane, hydrogen, carbon dioxide in liquid and gaseous phase) and 105 stoichiometric and kinetic parameters. The SIMBA 6.6 software package (ifak system GmbH, Germany), working in a 32-bit environment MATLAB/SIMULINK (MathWork, USA) was used as a simulation tool.

Identification of parameters

In the ADM1xp model, anaerobic digestion is divided into four basic processes. Each of them is described by specific kinetics rate equations (Table 1). All biochemical extracellular processes are assumed to be the first order, whereas all intracellular reactions are Monod-type kinetics.

Model calibration and verification

In the present study, for calibration of ADM1xp, the genetic algorithm optimization procedure, *ga*, included in the MATLAB R2012b (MathWork, USA) package was used. Experimental results of biogas/methane production, pH, the concentration of acetate, propionate, and valerate in digestate were used. The first step was to set the initial values of all model parameters to

be the same as in Batstone et al. (2002). Then, simulations were performed to fit the model output. The following parameters were adjusted: disintegration constant (k_{dis}), maximum uptake rate for butyrate ($k_{m,c4}$), propionate ($k_{m,pro}$), acetate utilisers ($k_{m,ac}$), half saturation coefficients ($K_{S,c4}$), ($K_{S,pro}$), ($K_{S,ac}$) and the coefficients describing inhibitory effect ($K_{I\,h2,c4}$), ($K_{I,H2,pro}$), ($K_{I\,nh3}$). Other parameters have been used according to Batstone et al. (2002), without any modification.

The objective function, J_C, (eq. (1)) used to confirm the accuracy of ADM1xp. It was defined as the mean value of the squared differences between the experimental and estimated values of selected fractions (F):

$$J_C\left(\begin{array}{cc} model & coefficients \end{array}\right) = \frac{\sum_{i=1}^{n}\left(F_{i,\exp} - F_{i,\mathrm{mod}}\right)^2}{n} \qquad (1)$$

where, n, is the number of experimental points.

The values of the model coefficients were determined by solving the following optimization formula (eq. (2)):

$$\min J_C\left(\begin{array}{cc} model & coefficients \end{array}\right). \qquad (2)$$

In the present study, simulation of biogas production was calibrated by adjusting mainly disintegration constant (k_{dis}). The rest of the parameters were slightly modified to obtain proper fitting of experimental to simulated data. Next, for the estimated value of $k_{dis,}$ the values of kinetic parameters of VFAs uptake were optimized.

Model's verification was based on logical assessment of ADM1xp correctness. Simulated values of variables were analyzed with literature data for compliance with theoretical assumptions and values of kinetic coefficients in the ADM1xp.

Results and discussion

Estimation of parameters in the ADM1xp

Disintegration and hydrolysis

Degradation of particulate organic matter in the ADM1xp is divided into two steps: disintegration and hydrolysis. The degradation of material with lumped characteristics (referred to as composite), starts from disintegration, while hydrolysis is related to well defined substrates, such as carbohydrates, proteins and lipids. ADM1xp assumes a low rate of disintegration (k_{dis} = 0.5 d^{-1}) and high hydrolysis constants for k_{hydch}, k_{hydpr} and k_{hydli} (10 d^{-1}) (Batstone et al. 2002).

The values of initial and final parameters for disintegration and hydrolysis are given in Table 2. During calibration of ADM1xp, the first order parameters for disintegration rate turned out to be lower than the initial values given by Batstone et al. (2002), indicating a slower breakdown of the composite material (X_c). The parameters for hydrolysis

Table 1. Processes in anaerobic digestion and numbers of kinetic rate equation

Group	Process	Number of kinetic rate equations (ρ)	Number of parameters
1	disintegration	1	1
	hydrolysis	2–4	4
		13–19	
2	acidogenesis	5–6	8
3	acetogenesis	7–10	12
4	methanogenesis	11–12	12

Table 2. Values of biochemical parameters for a mixture of maize silage and cattle manure during disintegration and hydrolysis

No.	Parameter	Unit	Initial value*	This study	Literature values
1	k_{dis}	d^{-1}	0.5	0.1	0.26 for grass ensilage (Wichern et al. 2009) 0.001 for olive mill waste with phenol compounds (Fezzani and Ben Cheikh 2009) 0.5 for agricultural waste and manure (Wett et al. 2006) 0.006 for olive mill wastewater and solid waste (Boubaker and Ridha 2008) 0.15 for agro-residues (Galí et al. 2009)
2	$k_{hyd,ch}$	d^{-1}	10	10	0.025–0.20 for different particular substances (Christ et al. 2000)
	$k_{hyd,pr}$	d^{-1}	10	10	0.015–0.075 for different particular substances (Christ et al. 2000)
	$k_{hyd,li}$	d^{-1}	10	10	0.005–0.01 for different particular substances (Christ et al. 2000)
	k_{hyd}*	d^{-1}	10	–	0.009–0.094 for crops and crops residues (Lehtomaki et al. 2005) 0.94 for corn stover (Hu and Yu 2005) 0.31 for cattle manure + TMR** (Lübken et al. 2007) 0.266 for grass silage (Veeken and Hamelers 1999)

* adopted from Batstone et al. (2002)
** TMR – 43% corn silage, 18% gramineous silage, 12% crop groats, 9% water, 7% soy pellets, 7% cow grain, 4% hay

of carbohydrates, proteins and lipids were the same as the original values in the ADM1 and amounted to 10 d^{-1}.

The kinetic constants of disintegration estimated by different authors for composite material (X_c) varies significantly and depends on substrate type. Wichern et al. (2009) obtained k_{dis} = 0.26 d^{-1} for untreated grass silage in a continuous flow reactor. Biernacki et al. (2013) using the respirometric tests determined disintegration kinetic constant for cattle manure as 0.26 d^{-1}, and much higher k_{dis} for grass silage and maize silage; 1.7433 d^{-1} and 0.7705 d^{-1}, respectively. Veeken and Hamelers (1999) reported that k_{dis} values for grass varied between 0.033 d^{-1} and 0.266 d^{-1}. From literature review, data of disintegration kinetic for mixed substrates are uncommon. In our study, k_{dis} for mixture of manure and maize silage was 0.1 d^{-1}. This can be explained by a higher content of straw in manure used in this experiment.

After disintegration of the composite (X_c), the hydrolysis of proteins, lipids and carbohydrates proceeded at the same high rate suggested by Batstone et al. (2002). Summarizing, during anaerobic digestion of maize silage and cattle manure mixture, disintegration limited the rate of hydrolysis.

The literature data shows that in modeling of an anaerobic digestion, disintegration is omitted, assuming that feedstock contains mainly proteins, lipids and carbohydrates. In that case, the process starts from hydrolysis at much lower rate constants (0.009–0.94 d^{-1}). The values of hydrolysis parameters depend on substrate type (Table 2), because individual components in the substrate are hydrolyzed at different rates. For example, the hydrolysis of starch and hemicelluloses is faster than cellulose. Due to the higher structural complexity, hydrolysis rates for proteins can be lower than for carbohydrates or lipids (Bischofsberger et al 2005).

Acidogenesis

Acidogenesis is a microbial process including degradation of soluble sugars and aminoacids into simpler products. This is the fastest step of the anaerobic conversion of complex organic matter. Thus, changes in acidogenic rate constants do not influence the methane production rate (Vavilin et al. 1996). The parameters for this step are tabulated in Table 3. In the present study the parameters suggested for acidogenesis by Batstone et al. (2002) and Rosén and Jeppsson (2006) were set as the initial values in the ADM1xp.

According to Batstone et al. (2002) this group of parameters is characterized by little or no sensitivity of model outputs to parameter changes, which was confirmed by our investigations (Tab. 3).

One of the most important processes in the ADM1xp is the decay of biomass, responsible for producing particulate organic matter. In our study k_{dec} was the same as in the original ADM1 and amounted to 0.02 d^{-1}. However, the literature indicates that the first order decay rate can be differential. For example, for microorganisms degrading amino acids, it ranges widely between 0.1 and 6.1 d^{-1}, whereas for microorganisms oxidizing sugars from 0.01 to 3.2 d^{-1} (Angelidaki et al. 1998, Batstone et al. 2000, Batstone et al. 2002).

Acetogenesis

In acetogenesis, organic acids are converted to acetate, CO_2 and H_2O. In the ADM1, three acetogenic bacteria groups are included, which utilize long chain fatty acids, propionate and valerate/butyrate as substrates (Batstone et al. 2002). Propionate and acetate have been generally regarded as the most important intermediates in anaerobic digestion, and as major indicators of process imbalance. Despite this, the values for biokinetic parameters are still rarely found in literature. Table 4 gives initial and final values of estimated parameters such as: maximum substrate uptake rate (k_m), half-saturation constant (K_S), hydrogen inhibition constant (K_I) and decay rate constant (k_{dec}).

In the present study, the uptake rate for butyrate ($k_{m,c4}$) was the same, and lower for propionate ($k_{m,pro}$) compared to the values given in Batstone et al. (2002). The uptake rate of propionate has also been modified by other authors (Tab. 4). Angelidaki et al. (1999) used a propionate uptake rate of $k_{m,pro}$ = 5.5 d^{-1} describing fermentation of manure mixed with oil (Wichern et al. 2009). Similar results ($k_{m,pro}$ = 5.5 d^{-1} and $K_{S,pro}$ = 0.392 kg COD m^{-3}) were obtained by Lübken et al. (2007).

In our investigations, proper fitting of experimental data to ADM1xp required a decrease in the value of $K_{I\,h2,pro}$ for propionate degraders. Therefore, this can indicate that in biogas plants using agricultural waste and plant biomass, propionate-utilizing microorganisms show higher sensitivity than in systems with activated sludge under anaerobic conditions. The results of inhibition obtained in the present study are in agreement with results given by Koch et al. (2010)

Table 3. Values of biochemical parameters for a mixture of maize silage and cattle manure during acidogenesis

No.	Parameter	Unit	Initial value*	This study
1	$k_{m,su}$	d^{-1}	30	30
2	$K_{S,su}$	kg COD m^{-3}	0.5	0.5
3	$k_{dec,Xsu}$	d^{-1}	0.02	0.02
4	$pH_{UL,a}$	–	5.5	5.5
5	$pH_{LL,a}$	–	4	4
6	$k_{m,aa}$	d^{-1}	50	50
7	$K_{S,aa}$	kg COD m^{-3}	0.3	0.3
8	$k_{dec,Xaa}$	d^{-1}	0.02	0.02

* adopted from Batstone et al. (2002)

and Wichern et al. (2009). Both authors proposed much lower values of $K_{I,H2}$ for propionate and butyrate uptake (Tab. 4).

Methanogenesis

The methane-forming bacteria can be classified into hydrogen- and acetate-utilising methanogens. The second group of bacteria has 2–4 times lower growth rates than bacteria converting hydrogen (Bischofsberger et al. 2005). Despite this, about 70% of methane is produced with the first group of bacteria.

Methanosarcina and *Methanosaeta* genera participate in methane production from acetate. Differences of acetate uptake kinetics result in lower half saturation constants (K_S), maximum specific growth rates (μ_{max}) and acetate threshold concentrations for *Methanosaeta* spp. than for *Methanosarcina* spp. This is the main reason why *Methanosarcina* spp. is often found in environments with acetate concentration higher than 1 mM. In biogas reactors treating organic industrial waste mixed with manure, *Methanosarcina* spp. were mostly identified (Mladenovska and Ahring 2000).

It is commonly known that $k_{m,ac}$, K_{Sac} and pH_{ULac} are characterized by significant sensitivity under steady-state conditions and by critical sensitivity under dynamic conditions (Batstone et al. 2002). The initial and final values of the growth rates for methanogenes are shown in Table 5. Our investigations showed that the maximum uptake rate of acetate compared to the initial values, whereas the half-saturation constant was higher. The values obtained in the present study were comparable with data given by Boubaker et al. (2008).

Wichern et al. (2009) reported that the best fittings of experimental to simulated data were obtained for acetate uptake at $K_{I,nh3}$ = 0.0084 kmol m^{-3}, other parameters were kept as original given by Batstone et al. (2002). In our investigations, the use of lower value of $K_{I,nh3}$ (0.0026 kmol m^{-3}) allowed us to obtain initial value of $k_{m,ac}$. The growth kinetics of thermophilic strains of *Methanosarcina* spp. from full-scale thermophilic biogas plants were examined by Mladenovska and Ahring (2000). The μ_{max} values of the six isolates ranged from 1.056 to 1.536 d^{-1}, the $K_{S,ac}$ from 0.4173 to 1.59 kg COD m^{-3}. The $k_{m,ac}$ values ranged from 15 to 75 kg COD kg^{-1}COD d^{-1}. The authors concluded that the strains isolated from plants treating animal manures mixed with industrial organic wastes had a higher affinity for acetate than these strains isolated from reactors operating solely on manures.

In summary, Batstone et al. (2002) classified some parameters as the most sensitive under steady-state conditions and critically sensitive under dynamic conditions. Namely: the disintegration rate (k_{dis}), the hydrolysis rate of carbohydrates ($k_{hyd,ch}$), the hydrolysis rate of proteins ($k_{hyd,pr}$), the maximum uptake rate acetate ($k_{m,ac}$), the half saturation coefficient of acetate ($K_{S,ac}$), and the upper pH limit (pH_{ULac}). In our investigations, the initial values of the parameters, which required adjustment were: k_{dis} (to a lower value), $k_{m,ac}$ (to a lower value) and $K_{S,ac}$ (to a higher value). In addition, some parameters of the acetogenesis process, i.e. uptake rate of propionate and butyrate were changed.

Model verification

In the present study, the simulated results were compared to the experimental measurements of biogas/methane production, the effluent pH, concentrations of COD and fatty acids (acetate, propionate and valerate). The results of simulation are presented in Fig. 1. The accuracy of the ADM1xp predictions was confirmed by J_C (eq. 1) coefficient, which were as follows: biogas production (211), $\%CH_4$ (7.8), pH (0.03), acetate (0.098), propionate (0.089) and valerate (0.003).

The lower J_c value, the better fitting of simulated to experimental data. In the present study, high value of the J_c for biogas production resulted from its fluctuations during the experiment. Similarly, according to Lübken et al. (2007) at OLR 3.2 kg VS m^{-3} d^{-3}, the average biogas production was 3.58 m^3 d^{-1} with fluctuations from 1.97 m^3 d^{-1} to 5.72 m^3 d^{-1}.

Table 4. Values of biochemical parameters for a mixture of maize silage and cattle manure during acetogenesis

No.	Parameter	Unit	Initial value*	This study	Literature values**			
					Antonopoulou et al. (2012)[a]	Lübken et al. (2007)[b]	Wichern et al. (2009)[c]	Koch et al. (2010)[d]
1	$k_{m,fa}$	d^{-1}	6	6				
2	$K_{S,fa}$	kg COD m^{-3}	0.4	0.4				
3	$K_{I\,h2,fa}$	kg COD m^{-3}	5.0E-06	5.0E-06				
4	$k_{dec,Xfa}$	d^{-1}	0.02	0.02				
5	$k_{m,c4}$	d^{-1}	20	20	9.1	13.7		
6	$K_{S,c4}$	kg COD m^{-3}	0.2	0.23		0.357		
7	$K_{I\,h2,c4}$	kg COD m^{-3}	1.0E-05	1.0E-08			5.4E-08	5.0E-08
8	$k_{dec,Xc4}$	d^{-1}	0.02	0.02				
9	$k_{m,pro}$	d^{-1}	13	8.5		5.5		
10	$K_{S,pro}$	kg COD m^{-3}	0.1	0.15		0.392		
11	$K_{I\,h2,pro}$	kg COD m^{-3}	3.5E-06	2.4E-08			4.8E-08	4.6E-08
12	$k_{dec,Xpro}$	d^{-1}	0.02	0.02				

* adopted from Batstone et al. (2002); ** – given only values different than in Batstone et al. (2002);
[a] – for acidified sweet sorghum extract; [b] – for cattle manure + TMR (43% corn silage, 18% gramineous silage, 12% crop groats, 9% water, 7% soy pellets, 7% cow grain, 4% hay); [c] – for grass silage; [d] – for grass silage

Table 5. Values of biochemical parameters for a mixture of maize silage and cattle manure during methanogenesis

No.	Parameter	Unit	Initial value*	This study	Literature values**					
					Antonopoulou et al. (2012)[a]	Lübken et al. (2007)[b]	Wichern et al. (2009)[c]	Koch et al. (2010)[d]	Fezzani and Ben Cheikh (2009)[e]	Boubaker and Ridha (2008)[f]
1	$k_{m,ac}$	d^{-1}	8	7.64	5.0	7.1		4.4		9.0
2	$K_{S,ac}$	kg COD m^{-3}	0.15	0.6						0.65
3	$K_{I\,nh3}$	kmole N m^{-3}	0.0018	0.00026			0.0084		0.0024	0.0028
4	$pH_{UL,ac}$	–	7	7		8	8.5			
5	$pH_{LL,ac}$	–	6	6						
6	$k_{dec,Xac}$	d^{-1}	0.02	0.02						
7	$k_{m,h2}$	d^{-1}	35	35						
8	$K_{S,h2}$	kg COD m^{-3}	7.0E-06	7.0E-06		3.0E-05	4.2E-05	5.6E-05		
9	$pH_{UL,h2}$	–	6	6						
10	$pH_{LL,h2}$	–	5	5						
11	$k_{dec,Xh2}$	d^{-1}	0.02	0.02						

* adopted from Batstone et al. (2002); ** – given only values different than in Batstone et al. (2002);
[a] – for acidified sweet sorghum extract, [b] – for cattle manure + TMR (43% corn silage, 18% gramineous silage, 12% crop groats, 9% water, 7% soy pellets, 7% cow grain, 4% hay), [c] – for grass silage, [d] – for grass silage, [e] – for olive mill waste with phenol compounds; [f] – for olive mill wastewater and solid waste

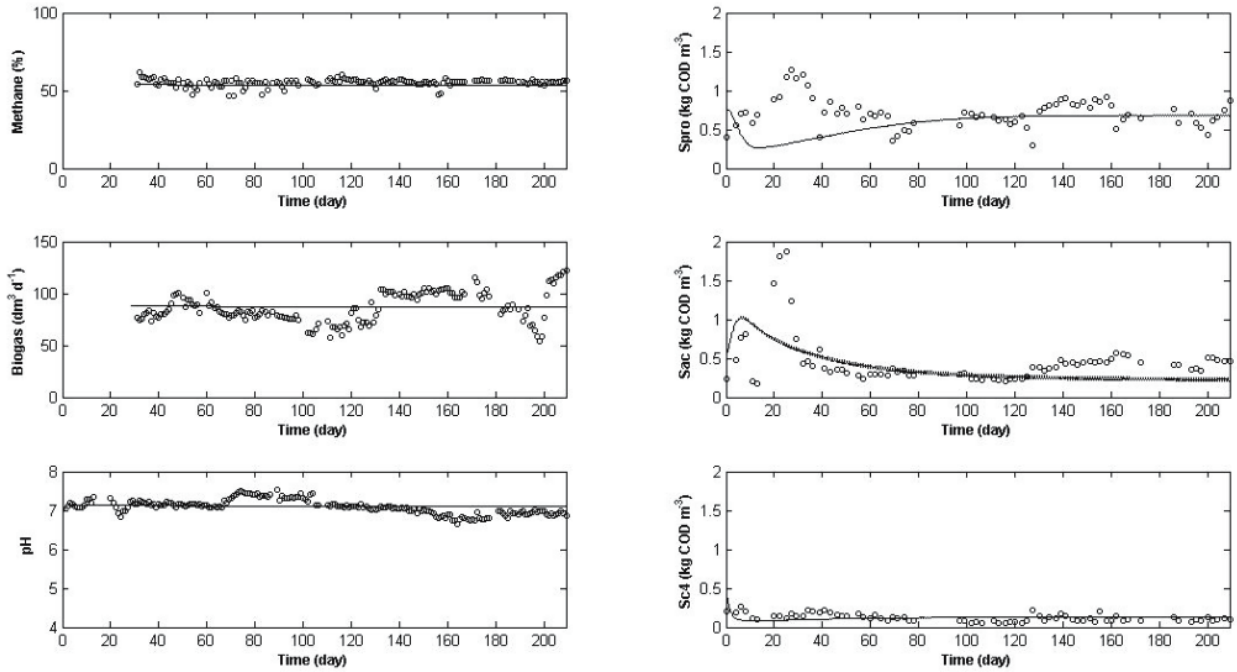

Fig. 1. The simulation of effluent pH, concentration of propionate (Spro), acetate (Sac) and valerate (Sva), biogas production and methane content in comparison with experimental data

Conclusions

1. Using the ADM1xp showed that the least satisfactory fitting of experimental to simulated data was for biogas production due to its fluctuations during the experiment, whereas the best were for propionate, butyrate and acetate.
2. The J_c function was used to evaluate the calibrate 9 among 105 kinetic parameters in the ADM1xp. The parameters for individual processes were: disintegration (k_{dis}), acetogenesis ($k_{m,c4}$; $K_{s,c4}$, $K_{I\,h2,c4}$, $k_{m,pro}$; $K_{S,pro}$; $K_{I\,h2,pro}$) and methanogenesis ($k_{m,ac}$; $K_{S,ac}$, K_{Inh3}).
3. The results of ADM1 calibration revealed that disintegration process proceeded slowly; k_{dis} = 0.1 d^{-1} and was 5-fold lower than the initial value.
4. The changes of kinetics parameters for VFAs uptake concerned mainly: propionate ($K_{I\,h2,pro}$ = 2.4·10^{-8} kg COD m^{-3}); butyrate ($K_{I\,h2,c4}$ = 1·10^{-8} kg COD m^{-3}) and acetate ($K_{S,ac}$ = 0.6 kg COD m^{-3}, $K_{I\,nh3}$ = 0.00026 kmole N m^{-3}).

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Modelowanie kofermentacji kiszonki kukurydzy i obornika bydlęcego za pomocą ADM1 – kalibracja i weryfikacja modelu (część II)

Streszczenie: Celem pracy było wykorzystanie modelu ADM1xp do symulacji procesu kofermentacji kiszonki kukurydzy i obornika bydlęcego. Przydatność modelu oceniano wykorzystując dane z eksperymentu w skali laboratoryjnej. Badania prowadzono przy obciążeniu komory ładunkiem organicznym OLR = 2,1 gVS $dm^{-3} \cdot d^{-1}$ oraz hydraulicznym czasie zatrzymania wsadu w fermentorze, HRT = 45d. Z powodu dużej liczby parametrów w modelu ADM1xp, zastosowano procedurę, która umożliwia zmniejszenie liczby weryfikowanych parametrów podczas kalibracji. Najlepsze dopasowanie danych eksperymentalnych do modelowych uzyskano po weryfikacji 9 spośród 105 stechiometrycznych i kinetycznych parametrów. Wartości współczynnika dopasowania (J_C) zmieniały się w zakresie od 0,003 (kwas walerianowy) do 211 (produkcja biogazu).