

Use of ADM1 model to simulate the anaerobic digestion process used for sludge waste treatment in thermophilic conditions

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Abstract

ADM1 model of IWA is still applied to a pilot scale anaerobic digestion process for the treatment of the waste activated sludge originating from a municipal wastewater treatment plant. This operation is carried out in a digester of 500 L volume. It is operated at an average hydraulic retention time (HRT) of 20 days with an average organic loading rate (OLR) of 1.27 kgTVS/m³ day, at a temperature of 55 °C with an average gas production rate (GPR) of 0.39 m³/m³ day.

The aim of the present study was to compare the results obtained from the simulation with the experimental values. ADM1 makes use of the experimental results for the optimization of the different kinetic parameters values. Generally, the simulated results are in a reasonably good fit for pH, methane and carbon dioxide percentages, biogas volume, chemical oxygen demand (COD), and total volatile fatty acids (TVFA). However, deviations are shown with an underestimation for the soluble chemical oxygen demand (SCOD) and inorganic carbon (IC) and an overestimation of inorganic nitrogen (IN).

Key Words: ADM1, Simulation, Energy, Anaerobic digestion, Sludge waste

Introduction

Anaerobic digestion is used worldwide, particularly in Europe, for the treatment of numerous types of biodegradable wastes. This is confirmed by the important number of treatment plants using this process on an industrial scale during the past few years as reported by Mata-Alvarez et al. (2000).

In fact, anaerobic digestion of the organic fraction of the municipal solid wastes alone or combined with organic sludge can contribute efficiently to solid waste reduction and biogas production as described by many researchers such as Jewell (1979), Kayhanian and Tchobanoglus (1992), Vallini et al. (1992), and Cout et al. (1994). This process was used by Mace et al. (2003), Bolzonella et al. (2003a), and Bolzonella et al. (2005a) for solid waste treatment under mesophilic or thermophilic conditions. Various solid wastes were used such as organic solid wastes with or without wastewater treatment plant sludge by Kayhanian and Rich (1995) and Bolzonella et al. (2005b), cheese whey by Ergüder et al. (2001), agro-industrial wastewaters by Demirer et al.

(2000), grey water from vacuum toilets by Feng et al. (2006), cow wastes by Igoud et al. (2002), olive mill waste by Fezzani and Bencheikh (2007), etc.

Due to the importance of anaerobic digestion as a treatment process, different dynamic models were elaborated, such as the AM2 which was developed jointly by researchers of the INRA of Narbonne and the INRIA of Sophia-Antipolis in 2001 as reported by Olivier et al. (2001). It is based on experimental results obtained on the fixed bed reactor of the INRA of Narbonne. Mainly this model is made up of 2 steps: acidogenesis and methanogenesis corresponding to acido-acetogens and methanogens bacteria populations, respectively. As a more recent and elaborate model, the anaerobic digestion model n° 1 (ADM1), was developed by Batstone et al. (2002), an IWA group. It includes, as a first step, the disintegration of solid complexes (non-biological step) into carbohydrates, lipids, proteins and inert material (soluble and particulate inert). The second step is the hydrolysis process of the disintegration products under an enzymatic action to produce sugars, amino acids, and long chain fatty acids (LCFA), successively. Then amino acids and sugars are fermented to produce VFA, hydrogen, and carbon dioxide (acidogenesis). Then LCFA, *propionic* acid, butyric acid and valeric acid are under anaerobic conditions, oxidized into acetate, carbon dioxide, and hydrogen (acetogenesis). Finally, methane can be produced through 2 paths: the first one is based on acetate, whereas the second one is through the reduction of carbon dioxide by molecular hydrogen. The organic species and hydrogen, in this model, are expressed as COD, whereas inorganic nitrogen and inorganic carbon species are expressed through their molar concentrations.

Since its development in 2002 and up to now the ADM1 has been tested and used on different substrates where a great number of research works are reported in the literature. As examples, one can cite the study by Blumensaat and Keller (2005), who modified the initial version of ADM1 for the simulation of a dynamic behaviour of a pilot scale digester using sludge, in order to ensure a successful model implementation. They obtained accurate results for the cases of low to medium loading rates. However, the accuracy showed a decline with the increase of the loading rate.

Wayne and Parker (2005) considered the application of the ADM1 to a variety of anaerobic digestion configurations where the results showed, in most of the considered cases, that the model was able to reproduce the trends of the experimental results.

Feng et al. (2006) found that the ADM1 is not sensitive to the distribution ratio of carbohydrates, proteins, and lipids, whereas the fraction of short chain fatty acids (SCFA) in the influent is rather more important.

Wolfsberger and Halubar (2006) and Batstone and Keller (2003) brought extensions and modifications to ADM1 to enlarge its prediction capabilities by taking into account other factors such as the sulfato-reducers or the degradation of certain substrates.

Fezzani and Ben Cheikh (2009) brought extensions to ADM1 to include phenolic compounds biodegradation process for the simulation of anaerobic digestion of olive mill wastes under thermophilic conditions. Also, Ramirez et al. (2009) used a modified ADM1 disintegration/hydrolysis structure for modelling batch anaerobic digestion for thermally pretreated waste activated sludge under thermophilic conditions.

Finally Usama Zaher (2005) considered the toxic effects of cyanide as an inhibition process for acetate.

Consequently, the great capabilities of ADM1 in modelling and calculations involving different types of substrates have been the motivating factor for the present work to extend its use to the evaluation of the performances of a digestion process for the treatment of activated sludge waste in the above mentioned 500 L pilot reactor working at a thermophilic temperature of 55 °C.

Experimental

Experimental data were obtained from the monitoring of an anaerobic digestion of sludge waste obtained from a wastewater treatment plant, carried out in the above mentioned pilot digester and under fixed thermophilic conditions ($T = 55\text{ }^{\circ}\text{C}$). The reactor was continuously stirred (CSTR), without recycle. It is made of stainless steel (AISI 304) and is jacketed to ensure the appropriate heat transfer. It is equipped with a mechanical agitator and a heater of water circulating around the digester. The temperature was electronically controlled to ensure a deviation of $\pm 2\text{ }^{\circ}\text{C}$. It is daily fed with 22.5 L and mass loading of 1.2 kg TVS/m³/day of substrate composed of sludge obtained from wastewater treatment plant after the secondary tank in MLSS form to maintain a hydraulic retention time (HRT) of 20 days, during the entire experimental phase. The operating digester period was 3 months including the starting up phase. Daily influent and effluent analyses were performed for pH, total solids (TS), total volatile solids (VS), volatile fatty acids, biogas volume produced and its composition, partial alkalinity (TA) and total alkalinity (TAC), and ammoniacal nitrogen (NH₃). Other analyses were made 2 or 3 times a week, like chemical oxygen demand, total nitrogen Kjeldahl (TKN), and total phosphorous (P_{tot}).

Analyses of COD, TS, TVS, pH, bicarbonate alkalinity, NH₃, TKN, and P_{tot} were performed according to the standard methods for the Examination of Water and Wastewater (1998). Concerning TVFA were analysed by gas chromatography equipped with flame ionization detector (FID) and capillary column (15 m of length and diameter of 0.53 mm), with hydrogen as carrier gas (APHA, 1998). The biogas composition is obtained using a portable gas analyser (Geotechnical Instrument, MOD. GA2000) operating by IR detection. It gives directly the percentages of methane and carbon dioxide. It is also able to detect and measure the concentration of hydrogen sulphide in the biogas within a range of 1 to 5000 ppm. For the measurement of produced gas volume a hydraulic gas flow meter (Ritter) was used.

Results and Discussion

Experimental monitoring of the pilot scale reactor

The pilot scale anaerobic digester was monitored for 3 months. Typical characteristics of influent feed are shown in Table 1. This is the stream resulting from the waste activated sludge. The typical solids concentration was about 4% while TVS were 60% of TS.

The effluent characteristics are shown in Table 2. Total volatile solids were clearly reduced around 30% with respect to the influent and the effluent parameters shown in Tables 1 and 2, respectively. This percentage is equivalent to the reduced part of TVS and is calculated as the ratio of the difference between the mean TVS values of the influent and effluent over the mean TVS value of the influent. Values of alkalinity, pH, and VFA were stable enough with low fluctuations and similar to typical results reported by Bolzonella et al. (2003b).

Implementation of ADM1

The substrate (sludge waste) was characterized according to Batstone et al.'s (2002) original version of ADM1. Therefore, the input data were calculated on the basis of the influent substrate characteristics mentioned in Table 1. There are several parameters such as: COD, IC, IN, pH, Temperature, VFA, and Volume of digester. Thereafter, the ADM1 model was calibrated, using experimental data, through the optimisation of the different parameters, mainly the disintegration and hydrolysis ones, with a constraint on their values which should be within the physical range. The experimental and simulated results are discussed in the following paragraph.

Table 1. Influent characteristics.

Parameters	Middle	Minimum	Maximum	Standard deviation	Number of samples
pH	6.97	6.88	7.07	0.06	19
NH ₃ (mgN/L)	4.83	3.5	6.4	1	10
TKN (mgN/L)	40.00	6.6	47.5	13.6	9
TCOD (mg COD/L)	744.79	702.1	837.6	42.5	9
P _{tot} (mg P/gTS)	709.3	465.9	804.5	95.2	10
TS (g/L)	40.04	25.6	44.2	4.3	16
TVS (g/L)	24.13	14.9	27.2	2.8	16
TVS (%TS)	60.3	54.05	68.0	3.2	16
VFA (mg COD/L)	5.8	4.2	7.6	1.2	14
Partial alkalinity (mg CaCO ₃ /L)	175.3	136.6	201	20.9	19
Total alkalinity (mg CaCO ₃ /L)	302.9	241.2	370.9	38.1	19

Table 2. Effluent characteristics.

Parameters	Middle	Minimum	Maximum	Standard deviation	Number of samples
pH	7.78	7.7	7.89	0.05	19
NH ₃ (mg N/L)	4	4	4	0	2
TKN (mg N/L)	33.4	28.86	37	2.43	9
COD (mg COD/L)	20.3	18.3	23.3	1.96	9
P _{tot} (mgP/gTS)	748.4	653.6	851.6	82.1	10
TS (g/L)	31.80	25.35	35.23	2.70	16
TVS (g/L)	16.64	14.08	17.82	1.06	16
TVS (%TS)	52.54	46.67	59.26	3.67	16
VFA (mg COD/L)	16.59	4.01	39.11	9.93	18
Partial alkalinity (mg CaCO ₃ /L)	2152.4	1989.9	2440	137.8	19
Total alkalinity (mg CaCO ₃ /L)	3641.5	3396.9	3962.5	159.5	19

Table 3. Characteristics and biogas production.

Parameters	Middle	Minimum	Maximum	Standard deviation	Number of samples
Biogas volume (m ³ /day)	0.1772	0.111	0.236	0.03	13
Specific gas production (m ³ biogas /kgTVS)	0.33	0.75	0.44	0.05	11
Gas production rate (m ³ biogas /m ³ .day)	0.39	0.25	0.52	0.06	11
% CH ₄ (%)	64.44	61.3	67.8	1.69	13
% CO ₂ (%)	35.56	32.2	38.7	1.69	13
V-CH ₄ (m ³ /day)	0.1188	0.0529	0.1489	0.01	13
V-CO ₂ (m ³ /day)	0.0651	0.0529	0.0871	0.01	13
H ₂ S (ppm)	594	420	760	106.59	13

Estimation of kinetic parameter values Prior to the simulation step, the kinetics parameters concerning the disintegration and hydrolysis phases were first estimated, considering both experimental batch runs; i.e. sludge hydrolysis (batch tests in serum bottles were carried out to get an idea of the biodegradability and global hydrolysis rate constant) and the modelling of experimental data changing the values of the kinetic parameters. In particular, the ADM1 was first used to simulate experimental data obtained during the anaerobic digestion

runs. It was found that the adequate constants for disintegration and hydrolysis for this study were equal to typical values reported in the literature by Mata-Alvarez et al. (2003) as presented in Table 4. All the values of kinetics and stoichiometric constants were then maintained as in the ADM1 model.

Table 4. Initial and estimated values of kinetic parameters.

Kinetic parameters	Names	Units	Initial values used in ADM1	Initial values	Estimated values
K_{dis}	Disintegration constant	day ⁻¹	0.5**	0.7	0.5
$K_{hyd.Pr}$	Carbohydrate hydrolysis constant	day ⁻¹	10**	1.25*	2.0
$K_{hyd.Pr}$	Proteins hydrolysis constant	day ⁻¹	10**	0.5*	0.8
$K_{hyd.Li}$	Lipids hydrolysis constant	day ⁻¹	10**	0.4*	0.7

*Middle values obtained from Mata-Alvarez (2003)

**Values obtained from Batstone et al. (2003)

Simulation of the process and comparison with experimental data

After estimating the parameters of disintegration and hydrolysis of the substrate, the obtained results concerning the chemical oxygen demand both TCOD and SCOD as well as the TVFA are represented in Figure 1, where a quite good agreement with the experimental values can be noticed for the period up to the 15th day for TCOD and TVFA parameters. Thereafter, a deviation is shown between the 2 sets of values, i.e. experimental and simulated, for the TCOD. However, deviations are shown between both set of SCOD values, probably due to the particulate fraction of COD.

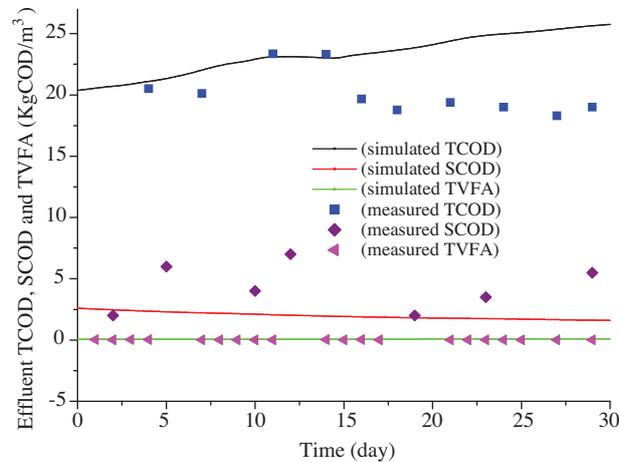


Figure 1. Comparison between the simulation and the experimental total and soluble COD and TVFA.

Moreover, the substrate distribution between proteins, carbohydrates, and lipids was not measured but default model values were adopted for this parameter. This can be justified by the fact that the experimental rig used is housed in the wastewater treatment plant and influent characteristics are varying daily. The reported values in the literature are specific to particular types of sludge waste, and hence may not be safely used in this work. However, the results concerning TVFA show a kind of good stability in the digester operations and fit reasonably well the experimental values.

Figure 2 shows the variation of the total gas volume produced with time, which clearly depends on the nature, composition, and biodegradability of the waste. In fact, even though the effective volume of the digester was

maintained almost constant, the amount of sludge could be different on any day, leading to different biogas production. Moreover, the structural limitations of the ADM1 imply that the simulated gas production follows an average path and therefore simulated data are only partially confounded with experimental values.

In order to have an insight on the biogas production the input organic loading rate was calculated and plotted as shown in Figure 2, where it can be seen that dynamic conditions are prevailing.

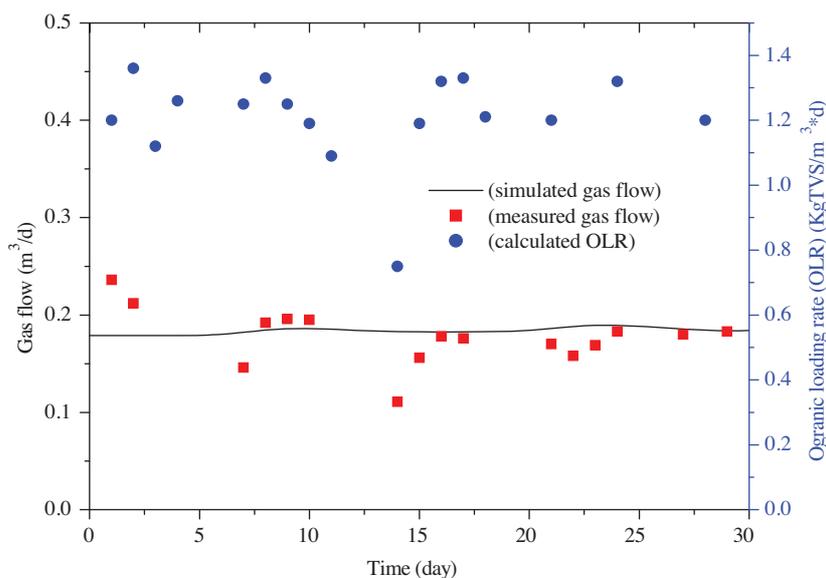


Figure 2. Comparison between the simulated and the experimental biogas production rate and the variation of the organic loading rate (OLR) with time.

Figure 3 shows the experimental and simulated results of gas production, which is composed of methane gas, carbon dioxide, and hydrogen. However, since the hydrogen volume is not important it was not analysed in the total volume and it was assumed that the gas is only made of methane and carbon dioxide. Even though this assumption could induce errors, the obtained results are satisfactory. At the beginning of the simulation, the results were overestimated for methane and underestimated for carbon dioxide. However, these results show that the reactor presented a good stability from the point of view of gas composition.

To see better what is happening in the system, IC, IN, and pH were represented in the same figure (Figure 4) and hence the alkalinity is implicit.

IC should be regarded as bicarbonate alkalinity (BA), since the variation of BA is due to the neutralisation of VFA in the solution. BA or IC are more sensitive to VFA accumulation than pH, and were empirically correlated to VFA accumulation by Bolzonella et al. (2003a). However, the variation of BA could not be converted into VFA units. From the simulation point of view ADM1 does not represent fluctuations but shows an average trend of the experiment (Figure 4).

The simulated results of inorganic nitrogen do not present the average experimental trend and seem to be overestimated compared to the experimental values (Figure 4).

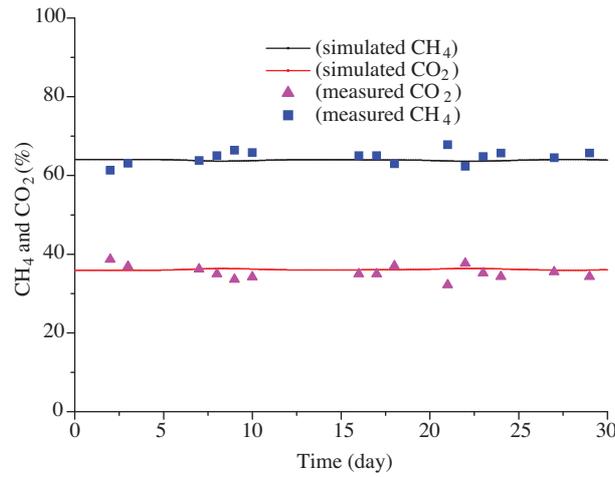


Figure 3. Comparison between the simulation and the experimental % (percentage) of CO₂ and CH₄.

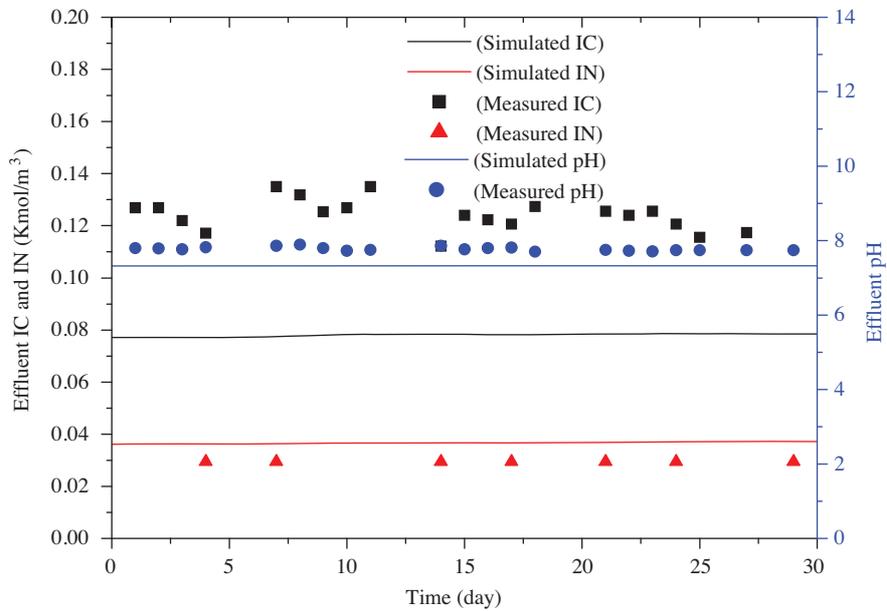


Figure 4. Comparison between the simulation and the experimental IC, IN, and pH.

The results of pH were underestimated by ADM1, but there are generally stable in comparison to BA variations (Figure 4). As a monitoring variable, BA was more sensitive than pH, and therefore it could be used as a control parameter for the operation of anaerobic digesters.

Conclusion

The ADM1 model was tested to simulate the behaviour of a bioreactor for the anaerobic digestion of activated sludge waste.

ADM1 showed acceptable simulating results, regarding the number of parameters involved and processes considered. However, it is important to note, according to the findings of this study, that the ADM1 model is used in simulating complex processes such as anaerobic digestion. In fact it cannot reproduce the intimate

variations of the different parameters, but an average trend is exhibited. This can be explained by the fact that not all the input kinetic parameters are obtained via analyses but extracted from the literature. In fact for hydrolysis and disintegration steps, the kinetic constant values first guesses were taken as the means of the ranges reported by Batstone (2002) in order to initiate their estimation within ADM1.

For the present case, the obtained experimental results can be tested for the prediction of different operating parameters. ADM1 can, therefore, be used as a managing tool of anaerobic digestion.

The simulated results show an acceptable fit. However, inorganic carbon or bicarbonate alkalinity is a very sensitive parameter to volatile fatty acids accumulation as shown by the variations of IC (Figure 4). This can be explained by the fact that IC is in this case in the form of BA, which is consumed to maintain the pH around neutrality in the digester. In order to improve the simulated results, substrate characterisation is necessary to avoid the use of default ADM1 parameters.

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