Modelling anaerobic digestion of sewage sludge: Mechanistic Models vs Machine Learning

M. S. Duarte[1,2], G. Martins[1,2], J.V. Oliveira[1,2], P. Oliveira[3], S. Silva[1,2], P. Novais[3], M.A. Pereira[1,2], M.M. Alves[1,2]

[1]CEB – Centre of Biological Engineering, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal
[2]LABBELS – Associate Laboratory, Braga, Guimarães, Portugal
[3]ALGORITMI – Centre, Department of Informatics, University of Minho, 4710-057 Braga, Portugal

(E-mail: salomeduarte@ceb.uminho.pt; gilberto.martins@deb.uminho.pt; jvoliveira@ceb.uminho.pt; pedro.jose.oliveira@algoritmi.uminho.pt; sergiosilva@ceb.uminho.pt; pjon@di.uminho.pt; alcina@deb.uminho; madalena.alves@deb.uminho.pt)

Abstract:

Anaerobic digestion processes are one of the technologies most used by wastewater treatment plants (WWTPs) to stabilize and decrease the organic content of sludge. This process decreases the costs of disposal while increasing the energetic efficiency of WWTPs. In order to optimize this process, three model approaches were implemented. First, we calibrated and validated the anaerobic digestion model no.1 (ADM1) using data from an anaerobic lab digester treating sewage sludge (Phases I, II, III), and further receiving glycerol pulses (Phases IV, V). Then, to optimize the calibration and parameter estimation, an iterative procedure was applied by minimizing the root mean square error (RMSE). The second approach consisted of applying a machine learning (ML) model to the biogas and methane produced. The results showed that the ADM1 model adjusted well to the experimental results, especially to biogas, methane and pH. The optimization routine was useful to identify the most sensitive parameters, improving model calibration. Overall, the ML approach was more reliable to predict anaerobic reactors' performance but did not respond so well to process perturbations (glycerol pulses).

Keywords: Anaerobic digestion; sewage sludge; mathematical modelling.

Introduction

The disposal of sludge generated during wastewater treatment may represent up to 50 % of the operating costs of a WWTP (Appels *et al.*, 2011). The implementation of anaerobic digestion (AD) is generally considered to be an economic and environmentally friendly technology to treat sewage sludge, since it allows to reduce the overall load of biosolids to be disposed, with simultaneous generation of a green energy carrier (biogas) (Appels *et al.*, 2011). The use of mathematical models in AD is a good way to design and assess the efficiency of anaerobic wastewater treatment, operational analysis, and control (Batstone *et al.*, 2006). This work aims to model the AD of sewage sludge (SS) under process perturbations. Two model approaches were implemented and compared: ADM1 was calibrated and validated; and a ML model was applied to the biogas and methane produced.

Material and Methods

Inoculum. Anaerobic granular sludge, from a WWTP of a brewery industry, was used as inoculum. It contained a volatile solids (VS) content of 82 ± 1 mg g^{-1} of sludge. The specific methanogenic activity in the presence of acetate (30 mmol L^{-1}) and H_2/CO_2

(80/20 v/v, 101.35 kPa) reached 145 ± 17 mL g^{-1} d^{-1} and 443 ± 26 mL g^{-1} d^{-1} (volume of methane produced at STP conditions per amount of VS of inoculum and time), respectively.

Substrates. SS was collected from WWTP (Braga, Portugal), after thickening and dewatering.

Reactors' operation. One anaerobic bioreactor was operated in mesophilic conditions (37 °C), with 4 L working volume and inoculated with anaerobic sludge (at a final VS concentration of 28.3 g L^{-1}). A semi-continuous system was adopted by feeding six times per week. The hydraulic retention time (HRT) was reduced from 40 d (Phase I) to 30 d (Phase II) and then to 20 d (Phase IIII), as presented in Table 1. In Phases IV and V macroalgae were added to the feeding together with SS (R1 and R2), and pulses of glycerol were added once a week only in R2.

Table 1. Operation conditions. The organic loading rate (ORL) is expressed in g of COD fed per L of working volume and per day.

Phase	**Time/d**	***HRT* / d**	***OLR* / (g L^{-1} d^{-1})**
I	1-51	40	1.58 ± 0.33
II	51-131	30	2.98 ± 0.76
III	131-179	20	3.38 ± 0.13
IV	179-220	20	3.74 ± 0.08 (Plus 8.83 pulse)
V	220-242	20	3.83 ± 0.00 (Plus 16.85 (pulse)

Analytical methods. TS, VS, pH, TKN were measured according to Standard Methods (APHA *et al.*, 1999). COD was determined using standard kits (Hach Lange, Düsseldorf, Germany). Volatile fatty acids (VFA) concentration and the % of methane in the biogas was measured following the guidelines in (Oliveira *et al.*, 2015).

Mechanistic model. ADM1. The ADM1 Matlab/Simulink implementation proposed by Rosen and Jeppsson, (2006) was used in the present study. In brief, ADM1 describes the different steps of AD: disintegration, hydrolysis, acidogenesis, acetogenesis, and methanogenesis (Batstone *et al.*, 2002), and considers 26 state variables and 19 biochemical reactions associated with 7 bacterial populations. More details about model description and model parameters can be found in Batstone *et al.*, (2002) and Rosen and Jeppsson, (2006). The major input variables driving the model are presented in Table 2. To calibrate the model, heuristic approach was followed intending to minimize the root mean square error (RMSE). 28 parameters were adjusted to fit experimental results (using the average data of the first 180 d of reactors operation). The values of the remaining model parameters were taken from Rosen and Jeppsson, (2006). Model validation was confirmed by comparing the simulated results with the data from reactor operation from day 180 to 240.

Machine Learning. To compare the mechanistic approach with the data-driven model, an Artificial Neural Network (ANN) was developed, namely a Recurrent Neural Network (RNN). RNNs have shown excellent performances in the context of time series forecasting in the literature due to their ability to create a memory of the data behaviour in this type of problem. Namely, in this study, we used a kind of RNNs, the Long Short-Term Memory (LSTMs).

Table 2. The major input variables driving the model.

Time / d	S_{IC}[1] / kmol·m^{-3}	S_{IN}[2] / kmol·m^{-3}	X_{xc}[3] / kg COD·m^{-3}	X_{li}[4] / kg COD·m^{-3}	X_I[5] / kg COD·m^{-3}	OLR / kg COD·m^{-3}·d^{-1}
0 - 50	0.060	0.074	57.9	0	11.6	1.0
50 - 90	0.080	0.074	69.5	0	13.9	1.3
90 - 119	0.080	0.234	81.1	0	16.2	4.1
119 - 131	0.080	0.127	68.9	0	13.8	2.2
131 - 155	0.060	0.127	50.2	0	10.0	3.3
155 - 180	0.060	0.124	66.2	0	13.2	3.2
180 - 210	0.060	0.300	74.1	93.6	18.75	8.5
210 - 220	0.060	0.304	95.5	163.7	25.05	8.6
220 - 234	0.060	0.528	105.2	231.0	28.05	15.5
234 - 241	0.060	0.519	106.4	228.2	28.35	15.2

[1] Concentration of inorganic carbon (bicarbonate concentration); [2] Concentration of inorganic nitrogen (NH_4 from macronutrients solution); [3] Concentration of composite materials (COD of sewage sludge); [4] Concentration of lipids (COD of crude glycerol); [5] Concentration of particulate inerts (estimated to be 20 % of composites)

Results and Conclusions

Phases I, II and III ended with a methane production yield (m^3 of methane per kg of VS consumed) of 0.47 m^3 kg^{-1}, 0.64 m^3 kg^{-1} and 0.49 m^3 kg^{-1}, respectively. Notice that a real digester of SS should produce 0.7 m^3 kg^{-1} (Grady *et al.*, 1999). Therefore, laboratory results for Phase II were the most similar to a real situation. The solids concentration increased constantly after day 20 and stabilised at 60 g L^{-1} for TS and 40 g L^{-1} for VS, during Phase III. In the end of Phase I, the VS reduction (VS_{red}) was 52 %. Phases II and III ended with a VS_{red} close to 43 %. In the intermittent addition of glycerol (R2) VS_{red} reached 48 % and 56 %, and the methane production yield (per VS) was 0.26 m^3 kg^{-1} and 0.31 m^3 kg^{-1}, in Phases IV and V, respectively.

Regarding model results, ADM1 responded very well in the prediction of biogas flow, methane proportion in the biogas, pH and dissolved COD. As an example of model calibration, Figure 1 depicts the simulated and experimental results for biogas flow (qgas). Contrary, simulated results for VFA, NH_4, and VS presented a significant deviation from the experimental results.

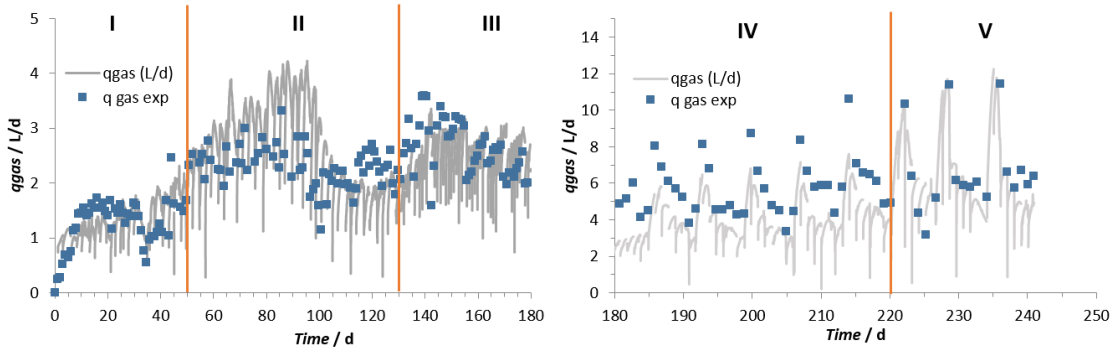

Figure 1. Example of model calibration (Phases I, II and III) and model validation (Phases IV and V).

To assess the quality of the optimised parameter sets and their applicability in the process model, a validation study was undertaken. The model outputs were compared with measured data from the Anaerobic Sequencing Batch Reactor treating sewage sludge and amended with crude glycerol. The process was simulated by applying the same implementation as described above and without changing the previously optimised parameter set. As observed in Figure 1 (IV and V), the biogas production responded as expected, i.e. increased with the glycerol pulses. COD also responded accordingly, as well as acetate accumulation. Simulated propionate and butyrate diverged from the experimental results, and these differences can be explained with the non-optimisation of several model parameters.

After calibration optimization the model results were improved. ML approach showed a better fitting with the experimental results from R1, indicating that these data-driven models could represent a good alternative to traditional mechanistic models. Nevertheless, with the ML model, the prediction of biogas flows in response to process perturbation (in this case glycerol pulses in R2) were not so accurate. Thus, future directions should couple both model approaches in hybrid models, incorporating the advantages of both models to predict and optimize anaerobic sludge bioreactors.

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