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A Scheme for Anaerobic Digestion Modelling and ADM1 Model Calibration

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Anaerobic digestion (AD) is a technology that produces biogas, also known as renewable natural gas, from organic waste materials under the activity of anaerobic microorganisms. In recent years, an increasing attention on energy produced from renewable resources has led to the need and development of tools helping with improving the process performance and design of AD, such as the Anaerobic Digestion Model No.1 (ADM1). ADM1 is a process-based model that can predict the biogas yield and identify potential prohibitions in the AD process from the properties of the feedstock and inoculum. Initial values of state variables and model parameters need to be calibrated when applying ADM1 to a particular feedstock. In this study, an ADM1 model using differential algebraic equations (DAE) system, called DAE ADM1, was developed. Specifically, the influence of the initial values of AD process state variables on the calibration of model stoichiometric and kinetic parameters were investigated, by comparing them with literature data, by highlighting their high impact on the model setup.

1. Introduction

Anaerobic Digestion (AD) is a process in which microorganisms degrade organic matter in the absence of air and produce biogas and digestate. The feedstocks for AD process can be sewage sludge, organic fraction municipal solid waste, manure etc., and the biogas produced is an important renewable energy. AD process offers environmental and economic benefits (Sahoo and Mani, 2019). AD process modelling plays an important role on AD plants design and operation optimisation (Fedailaine et al., 2015). Simulation results, in fact, allow a preliminary assessment of the process stability and biogas generation potential, with the possibility to easily analyse different co-digestion scenarios and operation conditions (Donoso-Bravo et al., 2011). The Anaerobic Digestion Model No.1 (ADM1) was developed by the International Water Association (IWA) AD Modelling Task Group (Batstone et al., 2002) to produce a generic model and common platform for dynamic simulations of AD processes. ADM1 is generally used for continuous stirred-tank reactors (CSTR), and includes 19 biochemical processes (describing reactions of disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis, plus three gas-liquid transfer processes and six acid-base kinetic processes). These processes describe conversions between 36 state variables (Table 1). On the basis of the study of Batstone et al. (2002), Rosen and Jeppsson (2006) successively developed the IWA benchmark simulation model 2 (BSM2) framework to link ADM1 with the activated sludge model (ASM), forming a plant-wide model for wastewater treatment plants. BSM2 has become a benchmark for studies using ADM1 because of the detailed description of the AD acid-base processes, together with the recommended values for model stoichiometric and kinetic parameters.
Numerous parameters are needed for ADM1 simulations, including input values of state variables related to the feedstock characteristics, initial values of state variables dependent on the inoculum characteristics and more than 100 model stoichiometric and kinetic parameters. These parameters need to be calibrated by experimental observations so that the model can describe and predict well the behaviour of an AD system treating a specific feedstock (Thamsiriroj and Murphy, 2011). However, long-term and regular tests of the digestate characteristics are usually lacking in the industrial AD systems, as they often require specific and high accuracy equipment (Yan et al., 2021). This has impeded the application of ADM1 model in industry.

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ADM1 input values can be roughly estimated by COD fractioning method from the particulate Chemical Oxygen Demand (COD) and soluble COD of the feedstock (Catenacci et al., 2021). For the determination of the stoichiometric and kinetic parameters when applying ADM1 to a specific feedstock, most parameters remain at the values provided in BSM2, and only about 10 sensitive parameters that have a large influence on model outputs will be calibrated. They can be decided through a sensitivity analysis (Nguyen, 2014; Thamsiriroj and Murphy, 2011). The calibration of these sensitive parameters to fit experimental data can be achieved either by heuristic manual adjustment (Nguyen, 2014) or by parameter optimisation algorithms (Baldé et al., 2020). In general, ADM1 studies listed the obtained values of sensitive stoichiometric and kinetic parameters from calibration, but most studies did not demonstrate how the initial values of state variables were determined and the specific values used, making published ADM1 modelling results hard to be replicated. Being ADM1 based on an ordinary differential equation (ODE) system, initial values of its state variables are crucial for the simulation outputs. The initial values, in fact, set how the ODE system iterations start, and they also affect the state variables increments at each time step. Additionally, the initial values of some state variables, such as the concentrations of the degrading bacteria, of hydrogen and methane dissolved in the liquid phase, are not easy to measure, and this is the main reason why they require to be calibrated together with stoichiometric and kinetic parameters by experimental data. However, when calibrating the model for multiple iterations by using the long-term running CSTR AD data, it can happen that the influence of possible inaccurate initial values becomes negligible (Arianna et al., 2021). In this case, the generic initial values, such as steady-state outputs from BSM2, can be used when calibrating the model for the first iteration. When data for model calibration are limited, initial values of stoichiometric and kinetic parameters become therefore important to achieve an effective AD processes prediction and a good system performance.

This paper investigates the effect of initial values on the calibration of the representative model parameters which can accurately predict the performance of the AD systems for a specific feedstock, especially when limited AD plant data are available for model calibration. Specifically, an ADM1 composed of differential algebraic equations (DAEs) was developed, called DAE ADM1, and verified via using BSM2 steady-state outputs. The influence of initial values was illustrated by reproducing the model calibration and validation stages results from a literature study (Nguyen, 2014).

2. Method

2.1 Anaerobic Digestion model structure

Standard ADM1 model simulates the AD process in CSTR reactors without recycling of digestate, by assuming that the bulk volume in the digester remains constant over time and inflow equals outflow (Batstone et al., 2002). The equation used in the DAE ADM1 code, describing the change of concentrations of soluble and particulate state variables with time, is shown in Eq(1).

$$\frac{dS(X)_{i,in}}{dt} = \frac{q^*S(X)_{i,in}}{V_{liq}} - \frac{q^*S(X)_{i,liq}}{V_{liq}} + \sum_{j=1\text{-}19} \rho_j v_{i,j} \quad (1)$$

where ρ_j is the kinetic rate for process j; $v_{i,j}$ is the stoichiometric coefficient for the state variable i in the reaction process j; q is the inflow and outflow, $S(X)_{i,in}$ and $S(X)_{i,liq}$ are the concentrations of the soluble or particulate state variable i in the inflow and in the reactor, respectively, and V_{liq} is the liquid phase volume in the reactor.

The ODEs for the acid-base kinetic processes for VFAs, inorganic carbon (IC) and inorganic nitrogen (IN) are implemented as suggested by Rosen and Jeppsson (2006). The term $\sum_{j=1\text{-}19} \rho_j v_{i,j}$ is added to the free form VFA, IC and IN, while the ODE describes the converting from the free form VFA, IC or IN to the base form VFA, bicarbonate or ammonia is described in Eq(2) (taking valerate as an example).

$$\frac{dS_{Va^-}}{dt} = -\kappa_{A/B\ Va} \cdot \left(S_{Va^-} \cdot S_{H^+} - K_{a,Va} \cdot (S_{Va} - S_{Va^-})\right) \quad (2)$$

where $\kappa_{A/B\ Va}$ is the acid-base kinetic constant of valerate and $K_{a,Va}$ is the acid dissociation constant of valerate. By assuming that the amount of gas components (S_{gas}) in the inflow (Table 1) was negligible, the ODEs describing the production of methane (CH_4) and carbon dioxide (CO_2) are shown in Eq(3) and Eq(4) (written as function of hydrogen, H_2).

$$\frac{dS_{gas,H_2}}{dt} = -\frac{q_{gas} \cdot S_{gas,H_2}}{V_{gas}} + \rho_{T,H_2} \cdot \frac{V_{liq}}{V_{gas}} \quad (3)$$

$$\rho_{T,H_2} = \kappa_L a_{H_2} \cdot \left(S_{H_2} - 16K_{H,H_2} \cdot p_{gas,\,H_2}\right) \quad (4)$$

where S_{gas,H_2} is the concentration of H_2 in the gas phase, while S_{H_2} is the concentration of H_2 in the liquid phase. V_{gas} is the volume of gas phase. $\kappa_L a_{H_2}$ is the overall gas-liquid mass transfer coefficient of hydrogen. $\kappa_L a_{H_2}$ is the Henry's Law constant for H_2. $p_{gas,\,H_2}$ is the partial pressure for hydrogen in the gas.

As discussed by Rosen and Jeppsson (2006), the ADM1 system can be 'stiff' because of the various time step variations of the different state variables reaction rates, which can vary from days for the biochemical processes to milliseconds for the pH. Implicit Matlab solvers can be adopted to stably solve stiff ODE systems without increasing the number of time steps to reduce the temporal discrepancies. However, the ability of these stiff solvers can be deteriorated when dealing with dynamic inputs (Rosen and Jeppson, 2006). Thus, a way to solve this problem, is to use the BSM2 suggestion to represent the two fast states, hydrogen ion (H^+) and H_2, by algebraic equations (DAEs) (i.e., Eqs(5) and (6)) and solve the DAE system by using explicit solvers, as considered in this study for the DAE ADM1 development. However, DAE ADM1 was coded by using Symbolic Math Toolbox and solved by 'ode15i' in Matlab – a variable step solver based on backward differentiation formulas (Shampine, 2002) and not in Simulink as for the BSM2 (Rosen and Jeppson, 2006).

$$S_{H^+} + S_{cat^+} + S_{NH_4^+} - S_{HCO_3^-} - \frac{S_{ac^-}}{64} - \frac{S_{pro^-}}{112} - \frac{S_{bu^-}}{160} - \frac{S_{va^-}}{208} - S_{OH^-} - S_{an^-} = 0 \quad (5)$$

$$\frac{q^*S_{H_2,in}}{V_{liq}} - \frac{q^*S_{H_2,liq}}{V_{liq}} + \sum_{j=1\text{-}19} \rho_j v_{i,j} = 0 \quad (6)$$

Table 1: Dynamic state variables in the ADM1 model.

Soluble				Particulate			
No.	Namee	Unit	Description	No.	Name	Unit	Description
1	S_{su}	kg COD/m^3	monosaccharides	22	X_c	kg COD/m^3	particulate
2	S_{aa}	kg COD/m^3	amino acid	23	X_{ch}	kg COD/m^3	carbohydrates
3	S_{fa}	kg COD/m^3	long chain fatty acid	24	X_{pr}	kg COD/m^3	proteins
4	S_{va}	kg COD/m^3	total valerate	25	X_{li}	kg COD/m^3	lipids
5	S_{bu}	kg COD/m^3	total butyrate	26	X_{su}	kg COD/m^3	sugar degraders
6	S_{pro}	kg COD/m^3	total propionate	27	X_{aa}	kg COD/m^3	amino acid
7	S_{ac}	kg COD/m^3	total acetate	28	X_{fa}	kg COD/m^3	LCFA degraders
8	S_{H_2}	kg COD/m^3	hydrogen in liquid	29	X_{c4}	kg COD/m^3	valerate and
9	S_{CH_4}	kg COD/m^3	methane in liquid	30	X_{pro}	kg COD/m^3	propionate
10	S_{IC}	kg COD/m^3	inorganic carbon	31	X_{ac}	kg COD/m^3	acetate degraders
11	S_{IN}	kmole N/m^3	inorganic nitrogen	32	X_{H_2}	kg COD/m^3	hydrogen degrader
12	S_I	kg COD/m^3	soluble inert	33	X_I	kg COD/m^3	particulate inert
13	S_{cat^+}	kmole/m^3	cation				
14	S_{an^-}	kmole/m^3	anion				
15	S_{va^-}	kg COD/m^3	base form valerate				
16	S_{bu^-}	kg COD/m^3	base form butyrate				
17	S_{pro^-}	kg COD/m^3	base form propionate				
18	S_{ac^-}	kg COD/m^3	base form acetate	Gas			
19	$S_{HCO_3^-}$	kmole C/m^3	bicarbonate	34	S_{gas,H_2}	kg COD/m^3	hydrogen
20	S_{NH_3}	kmole N/m^3	ammonia in liquid	35	S_{gas,CH_4}	kg COD/m^3	methane
21	S_{H^+}	kmole H^+/m^3	hydrogen ion	36	S_{gas,CO_2}	kmole C/m^3	carbon dioxide

2.2 Initial values influence identification

To verify the DAE ADM1 established in this study, the specific input data provided in BSM2 were considered (Table 2). Successively, the influence of initial values on stoichiometric and kinetic parameters calibration were investigated. Specifically, the initial values and model parameters calibrated by Nguyen (2014) to predict the AD performance of the model validation stage were used and results were compared with his study (Figure 1). Finally, this study also compared the model calibration stage results of Nguyen's (2014) (Table 3). As the initial values of this stage were not reported by the author, steady-state outputs from BSM2 were considered as initial values, which assumed that sewage sludge was used as inoculum material for the digester, with relative stable characteristics. The model parameters were kept at the calibrated value reported by the author (Nguyen, 2014).

3. Results

3.1 DAE ADM1 model verification

Table 2 and 3 show DAE ADM1 results and comparisons with literature studies for calibration.

Table 2: Steady-state simulation results of DAE ADM1 model against BSM2's ODE ADM1 model.

Soluble					Particulate				
No.	Name	BSM2	DAE ADM1	APE (%)	No.	Name	BSM2	DAE ADM1	APE (%)
1	S_{su}	0.0120	0.0120	0.00	22	X_c	0.3087	0.3087	0.01
2	S_{aa}	0.0053	0.0053	0.00	23	X_{ch}	0.0279	0.0279	0.00
3	S_{fa}	0.0986	0.0986	0.00	24	X_{pr}	0.1026	0.1026	0.00
4	S_{va}	0.0116	0.0116	0.00	25	X_{li}	0.0295	0.0295	0.00
5	S_{bu}	0.0133	0.0133	0.00	26	X_{su}	0.4202	0.4202	0.00
6	S_{pro}	0.0158	0.0158	0.00	27	X_{aa}	1.1792	1.1792	0.00
7	S_{ac}	0.1976	0.1812	**-8.30**	28	X_{fa}	0.2430	0.2430	0.00
8	S_{H_2}	0.0000	0.0000	0.00	29	X_{c4}	0.4319	0.4319	0.00
9	S_{CH_4}	0.0551	0.0533	**-3.18**	30	X_{pro}	0.1373	0.1373	0.00
10	S_{IC}	0.1527	0.1538	0.71	31	X_{ac}	0.7606	0.7612	0.08
11	S_{IN}	0.1302	0.1302	-0.00	32	X_{H_2}	0.3170	0.3170	0.00
12	S_I	0.3287	0.3287	0.01	33	X_I	25.6174	25.6174	0.00
13	S_{cat^+}	0.0400	0.0400	0.00					
14	S_{an^-}	0.0200	0.0200	0.00					
15	S_{va^-}	0.0116	0.0116	0.07					
16	S_{bu^-}	0.0132	0.0132	-0.01					
17	S_{pro^-}	0.0157	0.0157	-0.02					
18	S_{ac^-}	0.1972	0.1809	**-8.31**	Gas				
19	$S_{HCO_3^-}$	0.1428	0.1432	0.33	34	S_{gas,H_2}	0.0000	0.0000	-0.68
20	S_{NH_3}	0.0041	0.0039	**-5.45**	35	S_{gas,CH_4}	1.6256	1.5667	**-3.62**
21	S_{H^+}	0.0000	0.0000	**5.94**	36	S_{gas,CO_2}	0.014	0.0150	**6.27**

Table 3: Simulation results of DAE ADM1 model, compared with the model calibration stage in Nguyen's (2014).

Soluble					Particulate				
No.	Name	Nguyen	DAE ADM1	APE(%)	No.	Name	Nguyen	DAE ADM1	APE(%)
1	S_{su}	0.0049	0.0253	**416.04**	22	X_c	/	55.7374	***I***
2	S_{aa}	0.0022	0.0022	0.82	23	X_{ch}	0.2290	55.7374	**24239.50**
3	S_{fa}	0.0357	0.0356	0.19	24	X_{pr}	0.0132	1.3307	**9981.05**
4	S_{va}	0.0018	0.0008	**56.04**	25	X_{li}	0.0018	0.1532	**8411.12**
5	S_{bu}	0.0060	0.0024	**60.66**	26	X_{su}	8.0364	1.1788	**85.33**
6	S_{pro}	0.0061	0.0061	0.74	27	X_{aa}	0.3662	0.3690	0.75
7	S_{ac}	0.0285	0.0569	**99.64**	28	X_{fa}	0.0343	0.0296	13.66
8	S_{H_2}	0.0000	0.0000	**99.00**	29	X_{c4}	0.6878	1.4381	**109.08**
9	S_{CH_4}	0.0477	0.0467	2.15	30	X_{pro}	0.8091	0.6501	19.65
10	S_{IC}	0.1950	0.0494	**74.67**	31	X_{ac}	2.5956	0.625	**75.93**
11	S_{IN}	0.0800	0.0925	15.61	32	X_{H_2}	1.477	1.180	20.11
12	S_I	44.910	39.846	11.28	33	X_I	17.575	16.479	6.24
13	S_{cat^+}	0.0247	0.0250	1.22					
14	S_{an^-}	0.0659	0.0781	18.50					
15	S_{va^-}	0.0018	0.0008	**56.34**					
16	S_{bu^-}	0.0060	0.0023	**61.03**					
17	S_{pro^-}	0.0061	0.0060	1.81					
18	S_{ac^-}	0.0285	0.0564	**98.01**	Gas				
19	$S_{HCO_3^-}$	0.4785	0.0384	**91.97**	34	S_{gas,H_2}	0.0000	0.0000	7.29
20	S_{NH_3}	0.0650	0.0008	**98.76**	35	S_{gas,CH_4}	1.2507	1.3176	5.35
21	S_{H^+}	$3.1623*10^{-8}$	$1.4356*10^{-}$	**353.97**	36	S_{gas,CO_2}	0.0178	0.0163	8.52

Specifically, DAE ADM1 results were compared respectively with BSM2 (Rosen and Jeppsson, 2006) and Nguyen (2014) outcome and the absolute percentage errors (APEs) of the steady-state outputs were evaluated. In Table 2, the highest APEs (>1%) are related to the simulated concentrations of S_{ac}, S_{ac^-}, S_{NH_3} ($S_{NH_3} = S_{IN} - S_{NH_4^+}$), S_{H^+}, S_{CH_4}, S_{gas,CH_4} and S_{gas,CO_2}. Except for S_{CH_4}, S_{gas,CH_4} and S_{gas,CO_2}, they are all state variables in the algebraic equation for solving S_{H^+} concentration Eq(5). Since the DAE system is only an approximation of ODE system, this could be the source of the discrepancies of the APEs, as by influencing the following biogas production process, it can thus cause errors in the calculation of the gas concentrations of S_{gas,CH_4} and S_{gas,CO_2}. BSM2 study reported that the largest absolute error of steady-state simulation results between their DAE and ODE ADM1 models was only 10^{-5} (Rosen and Jeppsson, 2006). Another cause of DAE ADM1 errors could also be related to the implicit solver used in Matlab, which solves the non-linear equations by Newton's method (MathWorks, 2022).

3.2 Influence of initial values on DAE ADM1 model calibration

Results obtained by comparing DAE ADM1 with results of the model validation stage in Nguyen's (2014) are shown in Figure 1, respectively for pH (a), Total Ammonia Nitrogen (TAN) (b) and Acetic Acid (c). As shown, DAE ADM1 results, which are represented with a blue line, mostly match Nguyen (2014) simulation results, by considering the author's initial values and model parameters. Therefore, the stoichiometric and kinetic parameters calibrated by Nguyen (2014) can be considered representative for predicting the AD performance of his specific steady feedstock.

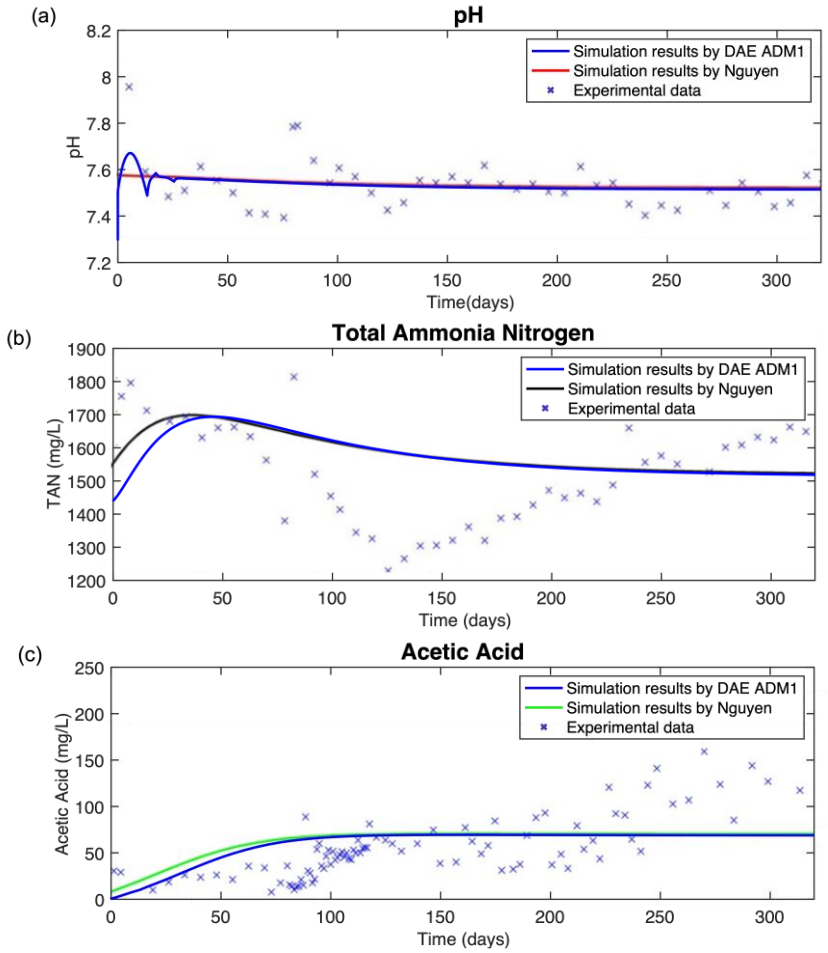

Figure 1. Comparison of the simulation results for pH, TAN and acetic acid of the model validation stage in Nguyen's (2014) study between his model and DAE ADM1.

As reported, the influence of the initial values on the calibration of model parameters was investigated by also reproducing the model calibration stage results in Nguyen's (2014) (Table 3). This further comparison aimed at verifying whether the same steady state simulation results could be obtained by using the generic initial values from BSM2 and the set of calibrated model parameters used above, or this set of representative model

parameters cannot be derived when calibrating the ADM1 using generic initial values. The steady-state outputs of Nguyen (2014) and DAE ADM1 are shown in Table 3, where half of the state variables differ by more than 50%, which prove the influence of generic initial values on the model performance. This could be attributed by Nguyen (2014) probably deriving the representative model parameters by iterative model calibrations and using long-term experimental data (which could make the influence of inaccurate initial values negligible, as previously explained in section 1), however this was not specified by the author. These results confirmed that if ADM1 is calibrated by using short-term experimental data as implemented in some studies (Baldé et al., 2020), it is crucial to provide a relatively accurate set of initial values, otherwise, the calibrated model is very unlikely to generate effective results for the model validation stage.

4. Conclusions

A DAE system ADM1 model was developed in this study, called DAE ADM1. Specifically, this model determined the concentrations of hydrogen ions ($H^{+)}$ and hydrogen (H_2) from anaerobic digestion processes by solving the main related equations via a DAE system. DAE ADM1 was verified by comparing its steady state outputs with results obtained from BSM2 framework and by comparison with literature studies. This study analysed the influence of the initial values of AD state variables on the calibration of the model stoichiometric and kinetic parameters. Results confirmed that the accuracy of the AD process initial values can be critical for an accurate prediction of the system performance. This study also highlighted the need of future work to develop an approach for ADM1 initial values and parameters calibration, when experimental observations are limited, as this is very common in industrial AD operations.

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