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Performance optimization and validation of ADM1 simulations under anaerobic thermophilic conditions

Nabil M. Atallah [a], Mutasem El-Fadel [a,*], Sophia Ghanimeh [b], Pascal Saikaly [c], Majdi Abou-Najm [a]

[a] Department of Civil and Environmental Engineering, American University of Beirut, Lebanon
[b] Department of Civil and Environmental Engineering, Notre Dame University – Louaize, Lebanon
[c] Water Desalination and Reuse Center and Division of Biological and Environmental Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia

HIGHLIGHTS

- ADM1 simulations of thermophilic anaerobic digesters treating food waste.
- Intermediary output influenced by different parameters depending on related processes.
- Methane-based calibration is less accurate in simulating intermediary by-products.
- Multiobjective optimization provided better overall results than methane optimization.
- Optimization results were validated upon their application on independent experiments.

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ABSTRACT

In this study, two experimental sets of data each involving two thermophilic anaerobic digesters treating food waste, were simulated using the Anaerobic Digestion Model No. 1 (ADM1). A sensitivity analysis was conducted, using both data sets of one digester, for parameter optimization based on five measured performance indicators: methane generation, pH, acetate, total COD, ammonia, and an equally weighted combination of the five indicators. The simulation results revealed that while optimization with respect to methane alone, a commonly adopted approach, succeeded in simulating methane experimental results, it predicted other intermediary outputs less accurately. On the other hand, the multi-objective optimization has the advantage of providing better results than methane optimization despite not capturing the intermediary output. The results from the parameter optimization were validated upon their independent application on the data sets of the second digester.

1. Introduction

Anaerobic digestion (AD) is a biological treatment process that involves a series of synergetic biochemical pathways that degrade organic matter into a methane-rich gas that can be used as a source of energy (Cesur, 2004). While it was initially applied in the treatment of liquid wastes with low solids content, its application evolved to targeting higher solid content wastes, such as food waste (El Fadel et al., 2012) albeit the drawback of system instability associated with the fast release of Volatile Fatty Acids (VFA) and high ammonia levels (Ghanimeh et al., 2013; Banks et al., 2008; Ward et al., 2008; Jeong et al., 2005). This problem is more pronounced in thermophilic systems where the high temperature (50–55 °C) increases degradation rates and speeds up the release of VFAs. As a result, long-term operation of thermophilic digesters, fed only with food waste, is often subject to instability and, in some instances, irreversible accumulation of inhibiting metabolic byproducts. In this context, the prediction of such disturbances and reduction of their occurrences become critical to a successful digester operation. For this purpose, the Anaerobic Digestion Model (ADM) series were developed by the International Water Association to test various biochemical reactions in the AD process including disintegration, hydrolysis, substrate uptake and decay, as well as physiochemical processes such as association/dissociation and liquid–gas transfer (Esposito et al., 2011). ADM1 has reportedly been successfully used in simulating AD of various types of waste, including, but not limited to, municipal waste, sewage

* Corresponding author at: American University of Beirut, Faculty of Engineering and Architecture, Bliss Street, PO Box 11-0236, Beirut, Lebanon. Fax: +961 1 744 462.
E-mail address: mfadel@aub.edu.lb (M. El-Fadel).

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sludge, manure and black water, and showed high correlation with experimental results (El Fadel et al., 2012; Kerroun et al., 2010; Wichern et al., 2009; Lee et al., 2009; BouBaker and Ridha, 2007; Jeong et al., 2005). Invariably, those applications rely on a set of data pertaining to one application using the final output (methane) to calibrate the model.

In this work, the ADM1 was applied for the first time to simulate the thermophilic AD of food waste using the performance data of four lab scale digesters. The simulation involved, in conjunction with a sensitivity analysis, parameter optimization and cross-validation against independent experimental data sets both at the intermediary by-products (pH, acetate, ammonia and Total COD), and final experimental output (CH_4-based results). To the best of our knowledge, no similar work has been reported in the literature.

2. Methods

2.1. Experimental program

Two anaerobic reactors (Bioflo 110, New Brunswick Scientific Co.) of 14 L capacity (9 L working volume) were fed with food waste collected from households and food markets, ground and homogenized with a lab food grinder, and characterized. The raw waste had a total solids content of 62–75 kg/m^3 and a COD of 96–120 kg/m^3.

Both reactors were operated at 55 °C and were continuously mixed with an internal impeller at 80 rpm. The digesters were fed with an equal batch of waste 3 times per week (Monday, Wednesday and Friday) resulting in the lowest daily loading rate over the weekend (Friday, Saturday and Sunday). Accordingly, a harmonic behavior of daily methane generation was observed with the lowest value being after Friday's feeding (i.e., on Saturday, Sunday and Monday). Wasting occurred at a volume of 700 ml to achieve a weekly average HRT of 30 days. The experiment lasted for 700 days and two separate sets of experimental data, with stable average weekly feeding rate, were selected for model calibration and validation:

Set 1 – Digesters A and B were run at a stable organic loading rate (OLR) of ~2.4 gVS/L/d for 115 days (days 376–491) and referred to as A1 and B1, respectively.

Set 2 – The digesters were run at a constant OLR of 2 gVS/L/d for 58 days (days 569–627) and the results are referred to as A2 and B2 for digesters A and B, respectively.

2.2. Experimental analysis

The temperature control was automated through a control unit connected to a built-in temperature probe and a heating blanket. The pH was continuously measured using a submerged pH probe and controlled by manual addition of NaOH (5 M) solution – when needed. Biogas measurements were taken once or twice daily, using the water displacement method for total gas yield and a dual wavelength infrared cell with reference channels (GEM-2000 monitor, Keison Products, UK) for CH_4 and CO_2 concentrations (% by volume). Biochemical analysis was conducted on a weekly basis whereby a fraction of the wasted material was used to measure total and volatile solids and total COD. Then, samples were centrifuged (4700 rpm, 10 min) and passed through filters with 1.2 μm openings for analysis of soluble solids, soluble COD, ammonia, and alkalinity. For VFAs, the filtrate was further passed through 0.2 μm syringe filter and acidified with phosphoric acid to pH of 2. The concentrations of acetate, propionate and butyrate inside the digesters were measured using a gas chromatograph (Trace GC Ultra, Thermo Electron corporation) equipped with a flame ionization detector and a TR-FFAP capillary column with nitrogen carrier gas.

COD (total and soluble) was determined using the modified 5220D procedure of Standard Methods for the Analysis of Water and Wastewater (APHA et al., 1998) by HACH high-range COD kit (HACH Company, Loveland, Colorado). Solid content (total, suspended, dissolved and volatile) was analyzed using Standard Methods (APHA et al., 1998) 2540B and 2540E procedures. Partial and total alkalinities (PA and TA, respectively) were measured by titration with HCl (0.2 N) to pH of 5.75 and 4.3, respectively. Total ammonia content was determined by spectrophotometry using HACH high-range ammonia kit (HACH Company, Loveland, Colorado).

Carbon and nitrogen content in the feed were determined using an organic elemental analyzer (Flash-1112 series EA, Thermo Finnigan). Total organic carbon in the feed was measured by combustion catalytic oxidation/NDIR technique using a dedicated TOC analyzer (TOC-V_{CSH} Total Organic Carbon Analyzer, Shimadzu Corporation, Japan). Total Phosphorous in the feed was measured using inductively coupled plasma mass spectrophotometry (Agilent 7500ce, EPA 200.8-3050).

2.3. Simulation process

The Anaerobic Digestion Model (ADM), developed by the International Water Association (IWA), was adopted in this study. The model ensures mass balance amongst various bacterial communities interacting with a heterogeneous substrate (Eqs. (1) and (2)) to represent transformation processes within the reactor boundaries.

$$\frac{dS_{liq,i}}{dt} = \frac{Q}{V_{liq}} \cdot (S_{in,i} - S_{liq,i}) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \quad (1)$$

where $S_{liq,i}$ = reactor concentration of soluble state variable i; Q = flow into and out of the reactor, m^3/day; V_{liq} = liquid reactor volume, m^3; $S_{in,i}$ = input concentration of soluble state variable I; $\Sigma\rho_{jvi,j}$ = the sum of the specific kinetic rate (ρ_j) of process j multiplied by the stoichiometric coefficients ($v_{i,j}$).

$$\frac{dX_{liq,i}}{dt} = \frac{Q}{V_{liq}} \cdot (X_{in,i} - X_{liq,i}) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \quad (2)$$

where $X_{liq,i}$ = reactor concentration of particulate state variable i; $X_{in,i}$ = input concentration of particulate state variable i.

In addition, acid-base equilibrium (Eq. (3)) is incorporated to simulate pH temporal profile and associated potential inhibition:

$$S_{Cat^+} + S_{NH_4^+} + S_{H^+} - S_{HCO_3^-} - \frac{S_{ac^-}}{64} - \frac{S_{pr^-}}{112} - \frac{S_{bu^-}}{160} - \frac{S_{va^-}}{208} - S_{OH^-} - S_{An^-} = 0 \quad (3)$$

where S_{ac^-}, S_{pro^-}, S_{bu^-}, S_{va^-}, $S_{NH_4^-}$ and $S_{HCO_3^-}$ are the concentrations of ionized forms of buffer components.

Also, liquid–gas transfer processes are considered (Eq. (4)) to determine biogas generation and composition:

$$\frac{dS_{gas,i}}{dt} = -\frac{q_{gas}}{V_{gas}} S_{gas,i} + \frac{V_{liq}}{V_{gas}} \rho_{T,i} \quad (4)$$

where $S_{gas,i}$ = gas phase concentration of gas component i; q_{gas} = gas flow outside the reactor; V_{liq} = reactor liquid volume; V_{gas} = reactor gas volume (headspace volume); $\rho_{T,i}$ = specific mass transfer rate of gas i.

The set of governing equations is solved simultaneously to simulate the dynamics and biological kinetics in the reactors. Details about model governing equations, input parameters, and underlying assumptions are described in Batstone et al. (2002).