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Application of Anaerobic Digestion Model No. 1 to describe the syntrophic acetate oxidation of poultry litter in thermophilic anaerobic digestion

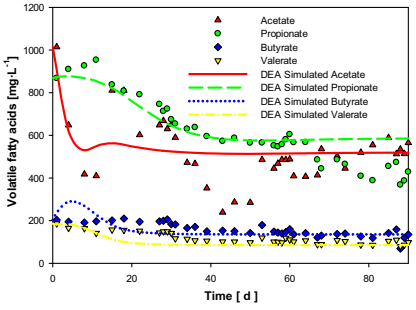
Víctor Rivera-Salvador [a], Irineo L. López-Cruz [b], Teodoro Espinosa-Solares [a,c,*], Juan S. Aranda-Barradas [d], David H. Huber [c,e], Deepak Sharma [c,e], J. Ulises Toledo [c]

[a] Departamento de Ingeniería Agroindustrial, Universidad Autónoma Chapingo, Chapingo, Estado de México 56230, Mexico
[b] Posgrado en Ingeniería Agrícola y Uso Integral del Agua, Universidad Autónoma Chapingo, Chapingo, Estado de México 56230, Mexico
[c] Gus R. Douglass Institute, West Virginia State University, Institute, WV 25112-1000, USA
[d] Unidad Profesional Interdisciplinaria de Biotecnología, Instituto Politécnico Nacional, Mexico City, DF 07340, Mexico
[e] Department of Biology, West Virginia State University, Institute, WV 25112-1000, USA

HIGHLIGHTS

- Hydrogenotrophic methanogens dominate poultry litter anaerobic digestion.
- Syntrophic acetate oxidation was modeled for poultry litter TAD.
- Differential evolution algorithms applied to evaluated ADM1 parameters.
- Evaluation of ADM1 syntrophic acetate oxidation kinetic parameters.

GRAPHICAL ABSTRACT



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ABSTRACT

A molecular analysis found that poultry litter anaerobic digestion was dominated by hydrogenotrophic methanogens which suggests that bacterial acetate oxidation is the primary pathway in the thermophilic digestion of poultry litter. IWA Anaerobic Digestion Model No. 1 (ADM1) was modified to include the bacterial acetate oxidation process in the thermophilic anaerobic digestion (TAD). Two methods for ADM1 parameter estimation were applied: manual calibration with non-linear least squares (MC-NLLS) and an automatic calibration using differential evolution algorithms (DEA). In terms of kinetic parameters for acetate oxidizing bacteria, estimation by MC-NLLS and DEA were, respectively, k_m 1.12 and 3.25 ± 0.56 kg_{COD} kg_{COD}^{-1} d^{-1}, K_S 0.20 and 0.29 ± 0.018 kg_{COD} m^{-3} and $Y_{ac\text{-}st}$ 0.14 and 0.10 ± 0.016 kg_{COD} kg_{COD}^{-1}. Experimental and predicted volatile fatty acids and biogas composition were in good agreement. Values of BIAS, MSE or INDEX demonstrate that both methods (MC-NLLS and DEA) increased ADM1 accuracy.

1. Introduction

Anaerobic digestion has the capacity for treatment of organic wastes and energy recovery via biogas as well as reduced CO_2 emissions and use of residues as fertilizer which make it a

* Corresponding author at: Departamento de Ingeniería Agroindustrial, Universidad Autónoma Chapingo, km 38.5 Carretera México-Texcoco, Chapingo, Estado de México 56230, Mexico. Tel.: +52 (595) 952 1730.
E-mail address: t.espinosa.s@taurus.chapingo.mx (T. Espinosa-Solares).

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sustainable technology (Shen et al., 2013; Zamanzadeh et al., 2013). Methane can be produced either by aceticlastic methanogens, which use acetate, or by hydrogenotrophic methanogens which utilize H_2 and CO_2. It has been reported that two thirds of methane produced by activated sludge derives from acetate whereas just one third is obtained from hydrogenotrophic methanogenesis (Boone et al., 1989).

Methanogenic acetate degradation is carried out by an aceticlastic reaction or an anaerobic syntrophic acetate-oxidizing reaction (Hattori, 2008; Westerholm et al., 2011). In conventional anaerobic digestion, acetate may be degraded by aceticlastic methanogens which limit the accumulation of acetate. In aceticlastic methanogenesis, acetate is cleaved to methyl and carboxyl groups; the methyl group is directly converted to methane by several biochemical reactions while the carboxyl group is oxidized to CO_2 (Hattori, 2008). However, an alternative pathway for acetate degradation involves a syntrophic relationship between acetate-oxidizing bacteria and hydrogenotrophic methanogens (Westerholm et al., 2011). This is known as syntrophic acetate oxidation.

Syntrophy is an essential intermediate step in the anaerobic conversion of organic matter to methane. In this mutualistic relationship, metabolically distinct microorganisms are tightly linked by the need to maintain the exchanged metabolites at very low concentrations (McInerney et al., 2009). Syntrophic metabolism requires reverse electron transfer, close physical contact and metabolic synchronization of the syntrophic partners (McInerney et al., 2009). Anaerobic digestion is also an expression of the syntrophic relationships among different microbes (Sasaki et al., 2011; Shen et al., 2013).

Syntrophic acetate oxidation is a two step methanogenesis from acetate by a coculture where acetate is oxidized to CO_2 and H_2 by one organism and H_2 is subsequently used by a second organism to reduce CO_2 to CH_4 (Westerholm et al., 2011). During the methanogenic mineralization process, syntrophic acetate oxidation is thermodynamically unfavorable ($\Delta G^{\circ\prime} = +104.6$ kJ mol^{-1}) (De Vrieze et al., 2012), and proceeds only if hydrogen partial pressures are kept low. By coupling hydrogen-consuming methanogens to the process, hydrogen partial pressures can be maintained between 10 and 40 Pa (72 ± 5 Pa in some cases) (Hao et al., 2011; Schink, 1997), and Gibbs free energies fluctuate near −20 kJ mol^{-1} (Hao et al., 2011). Thus, interspecies hydrogen transfer between secondary fermenting bacteria and hydrogenotrophic methanogens is important for the oxidation of substrates such as fatty acids, ethanol, propionate, butyrate and acetate (Hattori, 2008; Zamanzadeh et al., 2013).

Therefore, hydrogenotrophic methanogens play a crucial role in constantly removing H_2 and producing methane which makes the oxidation of substrate by proton reduction energetically feasible. Hence, the syntrophic association between substrate oxidizers and hydrogenotrophic methanogens is necessary for sustaining the overall process of anaerobic degradation (Luo et al., 2002). The acetate oxidation process is more common at thermophilic temperatures, although this process can also be developed at mesophilic conditions (Westerholm et al., 2010). However, if stress factors arise, ammonia accumulation for instance, aceticlastic methanogenesis can be inhibited (Schink, 1997; Wilson et al., 2012). There is a considerable difference in the acetate degradation rate for aceticlastic methanogenesis and syntrophic acetate oxidation which suggests that syntrophic acetate oxidation might be difficult to observe if both mechanisms are active at the same time (Schink, 1997).

There is also evidence that syntrophic acetate-oxidizing bacteria are important at high ammonia levels in thermophilic anaerobic digesters and high acid concentrations (Hao et al., 2011; Wilson et al., 2012). Acetate-oxidizing bacteria have been found to be important for the start-up of methanogenesis from high organic loadings in thermophilic anaerobic sequenced batch reactors (ASBR) at 55 °C (Hao et al., 2011). However, information about syntrophic acetate oxidation, the organisms involved, and their role in the methanogenic environment is currently limited, and more research is required to elucidate the kinetic and ecological characteristics of these bacteria (Hao et al., 2011; Westerholm et al., 2011). Recently, the microbial community structure of a pilot-scale thermophilic CSTR digester stabilized on poultry litter was characterized (Smith et al., 2014). Based on the predominance of hydrogenotrophic methanogens, as well as digester chemistry, bacterial acetate oxidation was proposed as the primary pathway for control of acetate levels in this digester.

Anaerobic Digestion Model No. 1 (ADM1) is a mechanistic model that explains complex substrates through their principal components (Batstone et al., 2002). It includes several steps that describe the biochemical and physicochemical processes involved in the anaerobic biodegradation of organic compounds. However, syntrophic acetate oxidation is not currently a part of the model but some suggestions have been made by Batstone et al. (2002) to take into consideration. Mathematical modeling has become a popular support tool for design, operation and control of activated sludge systems (Lübken et al., 2007). It can be used to predict process behavior in different situations and to assist operational management in order to develop strategies that will improve stability (Silva et al., 2009). These predictions can not only improve operational decision making in agricultural biogas plants but also assist the planning of research experiments (Zhou et al., 2011).

Because little progress has been made in the mathematical modeling of bacterial acetate oxidation (Shimada et al., 2011), the objective of this work was to incorporate bacterial acetate oxidation into a well-known mathematical model. The present paper simulates the TAD of poultry litter by incorporating the bacterial acetate oxidation pathway in ADM1 as the main acetate degradation process, rather than aceticlastic methanogenesis. Two methods for parameter estimation were used: differential evolution algorithms (DEA) and a coupled method of manual calibration and non-linear least squares (MC-NLLS).

2. Methods

2.1. Lab-scale digester

The digester that was used in this experiment was described as the control reactor in Sharma et al. (2013). This reactor was a 10 L glass vessel with a round-cylindrical bottom and separate ports for sampling, feeding and recirculation. The reactor was fed with a 2.2% TS chicken litter manure suspension during 90 days. The hydraulic retention time (HRT) was 15 days and the chemical oxygen demand (COD) was 24.77 ± 0.8 kg_{COD} m^{-3}. The feedstock was supplied at a semi-continuous rate of 0.66 L d^{-1}. The poultry litter (manure, feathers, and wood chips) was collected from Moorefield, WV and New Market, VA.

The mixing consisted of a digestate recirculation system without mechanical stirring. The digester was maintained at thermophilic conditions (56 °C) by running hot water through an external jacket. Temperature was monitored by a thermocouple. pH was automatically measured by a pH probe (Cole Parmer) connected in the re-circulation line. Biogas pressure was measured with a pressure transducer (Omegadyne Inc., model no. PX209-015G5V) when excess biogas was released into a cylinder containing water.

2.2. Analytical methods

For the substrate, total solids (TS) were determined using the standard methods of APHA (1998) and chemical oxygen demand