Recommendations for the accurate modelling of food waste anaerobic digestion

Gabriel Capson-Tojo, Renaud Escudié, Elie Desmond-Le Quéméner,
Jean-Philippe Steyer, Ángel Robles

Recommendations for the accurate modelling of food waste anaerobic digestion

Gabriel Capson-Tojo[1], Renaud Escudié[1], Elie Desmond-Le Quéméner[1], Jean-Philippe Steyer[1], Ángel Robles[2]

[1] INRAE, Univ Montpellier, LBE, 102 avenue des Étangs, 11100 Narbonne, France. e-mail: gabriel.capson-tojo@inrae.fr, renaud.escudié@inrae.fr, elie.le-quemener@inrae.fr, jean-philippe.steyer@inrae.fr

[2] Departament d'Enginyeria Química, Escola Técnica Superior D'Enginyeria, Universitat de Valencia, Avinguda de la Universitat s/n, 46100, Burjassot, Valencia, Spain. e-mail: angel.robles@uv.es

Highlights

- Syntrophic acetate oxidation and non-ideal ion speciation must be included
- Stoichiometry must be corrected as per food waste composition and amino acids
- Including chain elongation improved the butyrate and valerate predictions

Keywords: Syntrophic acetate oxidation; High-solids AD; Hydrogenotrophic methanogenesis; Ammonia.

Introduction

Efficient treatment and resource recovery from food waste (FW) is necessary for the implementation of sustainable and circular societies. Anaerobic digestion (AD) stands as an environmental-friendly and well-stablished technology to do so. Despite its potential, AD of highly concentrated substrates such as FW (20% total solids; TS) is a complex biological process prone to failure if not managed properly. Because of the fast biodegradability of FW, accumulation of volatile fatty acids (VFAs) has been frequently reported due to unbalance of the acidogenesis/acetogenesis and methanogenesis steps (Capson-Tojo et al., 2016). The high protein content of FW also leads to high concentrations of total and free ammonia nitrogen (TAN; FAN). FAN is toxic to microorganisms, mainly to strict acetoclastic methanogens (Capson-Tojo et al., 2018b, 2020). Thus, to accurately represent the AD of concentrated substrates such as FW, mechanistic models must consider the dominant metabolic pathways occurring (e.g. syntrophic acetate oxidation (SAO) and hydrogenotrophic methanogenesis (HM)) (Capson-Tojo et al., 2021). Furthermore, the TAN-FAN acid-base equilibria, which is affected, by pH, temperature, and by the high ionic strength of the media, must also be properly depicted (Capson-Tojo et al., 2020). A recent article proposed a modified version of the widely used ADM1 (Batstone et al., 2002) to include SAO and to accurately predict FAN concentrations using a modified Davies equation (Capson-Tojo et al., 2021). Results showed that these modifications were crucial to predict the system's behavior, particularly the acetate kinetics at reasonable uptake rates, and the accumulation of propionate (Capson-tojo et al., 2017). Nevertheless, the predictions for butyrate and valerate were far from perfect. This study aims at testing different alternatives that could further improve the predictions of these intermediates. More importantly, here we put together our previous knowledge to give recommendations that, in our opinion, are essential for an accurate modelling of FW AD.

Material and Methods

Batch results from Capson-Tojo et al. (2018a) were used to calibrate and validate the model. The different models compared were: (i) the unmodified ADM1 (Batstone et al., 2002), (ii) a modified ADM1 as in Capson-Tojo et al. (2021) (including SAO and non-ideal TAN-FAN equilibria) and including an accurate FW composition, (iii) model (ii) with uncoupled n-valerate and i-valerate consumption (as in Batstone et al. (2003)), (iv) model (ii) considering chain elongation for valerate production (from acetate, H_2 and propionate; assuming ethanol as non-detectable intermediate) and with a modified valerate stoichiometry from amino acid fermentation. To avoid biased comparisons, the modelling procedure was the same for all the approaches, as in Capson-Tojo et al. (2021). The simulations were carried out using MATLAB R2021a.

Results and Discussion

Even after calibration, the unmodified ADM1 (red line in Figure 1) was not able to accurately predict the results, mostly because SAO (the predominant acetate-consuming pathway) is not considered. In addition, the obtained values for the kinetic parameters related to acetotrophic growth and those for FAN inhibition were not realistic (Capson-Tojo et al., 2021). The modified ADM1 improved the performance considerably, but the butyrate and valerate profiles could not be accurately predicted simultaneously (either one profile or the other could be accurate, depending on the calibration done). Uncoupling n-valerate and i-valerate as in Batstone et al. (2003) did not enhanced the model

XIV Latin American Workshop and Symposium on ANAEROBIC DIGESTION — Juriquilla – Querétaro, 2023 — Anaerobic Digestion consolidating the Circular Economy

IWA the international water association

INSTITUTO DE INGENIERÍA UNAM

performance (results not shown). The modified model considering chain elongation allowed to uncouple the kinetics of butyrate and valerate uptake. The methane kinetics and acetate and propionate concentrations were again accurately predicted (as for model (ii)), but in this case the kinetics of butyrate and valerate were uncoupled, improving the accuracy of the predictions (further calibration efforts are needed and are currently being done). In the case of butyrate, its more accurate prediction was related to: (i) an accurate substrate fractionation in protein, carbohydrates and lipid contents (Capson-Tojo et al., 2017), and (ii) the uncoupling of the biomass responsible for butyrate an valerate degradation. Butyrate and valerate kinetics were very different, justifying this modification. Improving valerate predictions was more challenging. After trying several approaches, we found that including chain elongation in the model and reducing the amount of valerate initially produced from amino acid fermentation were necessary modifications to predict accurately the valerate profile. These modifications can be justified by: (i) the presence of traces of caproate in the reactors, confirming that chain elongation was indeed occurring, and (ii) the initial valerate kinetics differed totally from those of all the other VFAs, suggesting that its production was not related to the initial amino acid fermentation (the high soluble hydrogen concentrations in the first days would have inhibited valerate degradation, so no valerate consumption could occur). Chain elongation was included in the model assuming that the kinetics of ethanol production/consumption were much faster than those of valerate production, defining an overall reaction transforming acetate and hydrogen (ethanol precursors) and propionate (valerate precursor) into valerate.

Summarizing, considering SAO and non-ideal FAN-TAN equilibrium is crucial to accurately predict the methane production rates and the concentrations of acetate and propionate. Furthermore, if the concentrations of butyrate and valerate are to be predicted accurately, the substrate must be characterized and fractionated extensively, and chain elongation processes could be accounted for. Normally, butyrate and valerate do not represent a high proportion of the overall COD in the mass balance, but as they can act as indicators for AD instability, their accurate prediction is relevant.
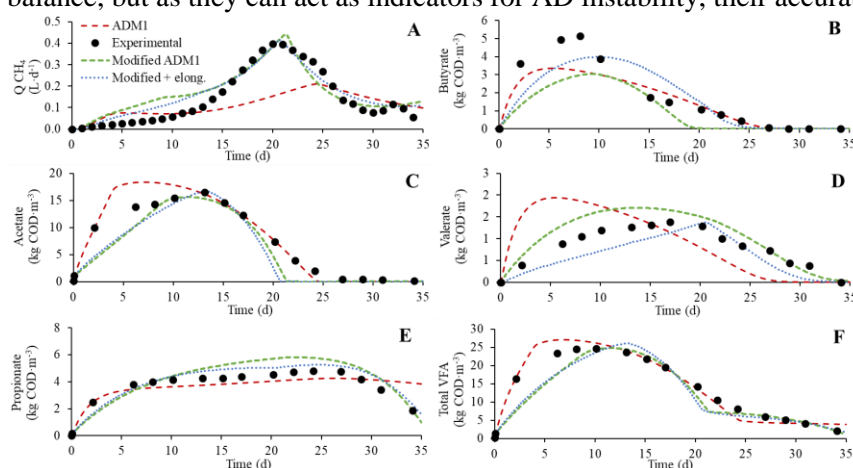
Figure 1. Experimental results and modelling results for (A) methane production rates and concentrations of (B) butyrate, (C) acetate, (D) valerate, (E) propionate, and (F) total VFAs.

References

Batstone, D.J., Keller, J., Angelidaki, I., Kalyuzhnyi, S. V, Pavlostathis, S.G., Rozzi, A., Sanders, W.T.M., Siegrist, H., Vavilin, V.A., 2002. The IWA Anaerobic Digestion Model No 1 (ADM 1). Water Sci. Technol. 45, 65–73.

Batstone, D.J., Pind, P.F., Angelidaki, I., 2003. Kinetics of Thermophilic, Anaerobic Oxidation of Straight and Branched Chain Butyrate and Valerate. Biotechnol. Bioeng. 884, 195–204.

Capson-Tojo, G., Astals, S., Robles, Á., 2021. Considering syntrophic acetate oxidation and ionic strength improves the performance of models for food waste anaerobic digestion. Bioresour. Technol. 341, 125802.

Capson-Tojo, G., Moscoviz, R., Astals, S., Robles, A., Steyer, J.-P., 2020. Unraveling the literature chaos around free ammonia inhibition in anaerobic digestion. Renew. Sustain. Energy Rev. 117, 109487.

Capson-Tojo, G., Moscoviz, R., Ruiz, D., Santa-Catalina, G., Trably, E., Rouez, M., Crest, M., Steyer, J.-P., Bernet, N., Delgenès, J.-P., Escudié, R., 2018a. Addition of granular activated carbon and trace elements to favor volatile fatty acid consumption during anaerobic digestion of food waste. Bioresour. Technol. 260, 157–168.

Capson-Tojo, G., Rouez, M., Crest, M., Steyer, J.-P., Delgenès, J.-P., Escudié, R., 2016. Food waste valorization via anaerobic processes: a review. Rev. Environ. Sci. Bio/Technology 15, 499–547.

Capson-Tojo, G., Ruiz, D., Rouez, M., Crest, M., Steyer, J.-P., Bernet, N., Delgenès, J.-P., Escudié, R., 2017. Accumulation of propionic acid during consecutive batch anaerobic digestion of commercial FW. Bioresour. Technol. 245, 724–733.

Capson-Tojo, G., Trably, E., Rouez, M., Crest, M., Bernet, N., Steyer, J.-P., Delgenès, J.-P., Escudié, R., 2018b. Methanosarcina plays a main role during methanogenesis of high-solids FW and cardboard. Waste Manag. 76, 423–430.