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Modelling anaerobic co-digestion in Benchmark Simulation Model No. 2: Parameter estimation, substrate characterisation and plant-wide integration

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ABSTRACT

Anaerobic co-digestion is an emerging practice at wastewater treatment plants (WWTPs) to improve the energy balance and integrate waste management. Modelling of co-digestion in a plant-wide WWTP model is a powerful tool to assess the impact of co-substrate selection and dose strategy on digester performance and plant-wide effects. A feasible procedure to characterise and fractionate co-substrates COD for the Benchmark Simulation Model No. 2 (BSM2) was developed. This procedure is also applicable for the Anaerobic Digestion Model No. 1 (ADM1). Long chain fatty acid inhibition was included in the ADM1 model to allow for realistic modelling of lipid rich co-substrates. Sensitivity analysis revealed that, apart from the biodegradable fraction of COD, protein and lipid fractions are the most important fractions for methane production and digester stability, with at least two major failure modes identified through principal component analysis (PCA). The model and procedure were tested on bio-methane potential (BMP) tests on three substrates, each rich on carbohydrates, proteins or lipids with good predictive capability in all three cases. This model was then applied to a plant-wide simulation study which confirmed the positive effects of co-digestion on methane production and total operational cost. Simulations also revealed the importance of limiting the protein load to the anaerobic digester to avoid ammonia inhibition in the digester and overloading of the nitrogen removal processes in the water train. In contrast, the digester can treat relatively high loads of lipid rich substrates without prolonged disturbances.

1. Introduction

The scope for wastewater treatment plants (WWTPs) has widened during recent years. Not only are the discharge limits getting stricter, also new constraints such as resource recovery, energy efficiency and mitigation of greenhouse gas emissions are being applied (Olsson, 2015). These issues increase the focus on energy recovery by anaerobic digestion (AD) at WWTPs. Many full-scale anaerobic digesters are oversized and therefore under-utilised (Lundkvist, 2005). Anaerobic co-digestion (AcoD) of organic wastes with sewage sludge allows the WWTPs to use residual digester capacity and thereby increase methane production and subsequently energy production (Batstone and Virdis, 2014; Mata-Alvarez et al., 2014). The application of AcoD at WWTPs is becoming more common and in the future is it likely that most medium to large size plants will practice AcoD. Even though the co-substrates are fed directly to the digester and not to the WWTP influent, it still produces an additional load on the WWTP water

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Nomenclature

AcoD	Anaerobic co-digestion
AD	Anaerobic digestion
ADM1	Anaerobic Digestion Model No. 1
ASM	Activated Sludge Model
ASM1	Activated Sludge Model No. 1
ASU	Activated sludge unit
B_0	Ultimate methane potential [m^3 CH_4 ton VS^{-1}]
BMP	Biomethane potential
BOD	Biological oxygen demand [kg O_2 m^{-3}]
BSM2	Benchmark Simulation Model No. 2
C_i	Concentration of substance *i* [kg m^{-3}]
COD	Chemical oxygen demand [kg O_2 m^{-3}]
COD_P	Particulate fraction of chemical oxygen demand [kg O_2 m^{-3}]
COD_s	Soluble fraction of chemical oxygen demand [kg O_2 m^{-3}]
COD_t	Total chemical oxygen demand [kg O_2 m^{-3}]
DAF	Dissolved air flotation
DO	Dissolved oxygen [kg O_2 m^{-3}]
EQI	Effluent quality index
f_d	Biodegradable fraction of total chemical oxygen demand [−]
γ_i	Conversion factor to COD for substance *i* (kg COD kg^{-1}).
GISCOD	General Integrated Solid Waste Co-Digestion model
I_{fa}	Long chain fatty acids inhibition (ADM1) [−]
I_{NH}	Ammonia inhibition (ASM1) [−]
ISS	Inorganic suspended solids
$K_{I,50}$	50% inhibitory concentration (ADM1) [kg COD m^{-3} d^{-1}]
$K_{i,fa,low}$	Parameter in long chain fatty acid inhibition (ADM1)
$K_{i,fa,high}$	Parameter in long chain fatty acid inhibition (ADM1)
k_{hyd}	Hydrolysis parameter (ADM1) [d^{-1}]
$k_{hyd,sludge}$	Hydrolysis parameter for sludge (ADM1) [d^{-1}]
LCFA	Long chain fatty acids
M_N	Molar mass of nitrogen [g.mol^{-1}]
NOx-N	Total nitrate and nitrite nitrogen [kg N m^{-3}]
OCI	Operational cost index
OLR_{ext}	Organic loading rate for co-substrates [kg COD m^{-3} d^{-1}]
OLR_{sludge}	Organic loading rate for sludge [kg COD m^{-3} d^{-1}]
PCA	Principal component analysis
$pH_{LL,ac}$	Lower limit of pH inhibition of uptake of acetate (ADM1)
Q_{gas}	Flow of biogas [m^3.d^{-1}]
Q_{CH4}	Flow of biomethane [m^3 CH_4 d^{-1}]
S_{aa}	Amino acids (ADM1) [kg COD m^{-3}]
S_{ac}	Total acetic acid (ADM1) [kg COD m^{-3}]
S_{bu}	Total butyric acid (ADM1) [kg COD m^{-3}]
S_{fa}	Fatty acids (ADM1) [kg COD m^{-3}]
S_I	Inert soluble organics (ADM1) [kg COD m^{-3}]
S_{IN}	Inorganic nitrogen (ADM1) (kmol m^{-3})
S_{pro}	Total propionic acid (ADM1) [kg COD m^{-3}]
S_{su}	Sugars (ADM1) [kg COD m^{-3}]
S_{va}	Total valeric acid (ADM1) [kg COD m^{-3}]
TAN	Total ammonia nitrogen [kg N m^{-3}]
TKN	Total Kjeldahl nitrogen [kg N m^{-3}]
TN	Total nitrogen [kg N m^{-3}]
TS	Total solids [kg m^{-3}]
TSS	Total suspended solids [kg m^{-3}]
VFA	Volatile fatty acids [kg m^{-3}]
VFA_t	Total volatile fatty acids [kg m^{-3}]
VS	Volatile solids [kg m^{-3}]
WWTP	Wastewater treatment plant
X_c	Composite material (ADM1) [kg COD m^{-3}]
X_{ch}	Carbohydrates (ADM1) [kg COD m^{-3}]
X_i	Inert particulate organics (ADM1) [kg COD m^{-3}]
X_{li}	Lipids (ADM1) [kg COD m^{-3}]
X_{pr}	Proteins (ADM1) [kg COD m^{-3}]

train. The organic matter in the co-substrate is degraded to a certain extent in the AD process and converted to biogas; however, mineralized nutrients are mobilised and recirculated to the water train. Therefore, one of the key factors for succeeding with AcoD is to select suitable co-substrate/s and their optimal dose rate. Co-substrate characteristics and applicability have been extensively reviewed by Mata-Alvarez et al. (2014). Ideal co-substrates will have a high methane potential, high degradable fraction (and minimum impact on residual solids production) and a nutrient composition suitably balanced for the host WWTP. Generally, this means that co-substrate characteristics will differ from those of WWTP sludges in terms of composition and degradation kinetics. While there are a large number of potential co-substrates suitable for treatment at WWTP, local substrate availability and transport costs will constrain the options for individual plants. Effective modelling of AcoD is a powerful tool to assess the resource efficiency, energy balance and plant-wide effects of various co-substrate feeds at a WWTP (Razaviarani and Buchanan, 2015).

To compare the performance of different control strategies in a unified framework the Benchmark Simulation Model No. 2 (BSM2) was developed (Gernaey et al., 2014). BSM2 represents a plant-wide model including digestion of sludge with the Anaerobic Digestion Model No. 1 (ADM1, Batstone et al., 2002). In light of the increased focus on digestion, it is important that the AD process is well described and allows modelling of common and developing applications, such as AcoD. However, the current standard implementation of ADM1 in BSM2 does not allow for addition of co-substrates or dynamic hydrolysis parameters. Furthermore, some important limitations in the AD related to AcoD common practice in WWTP are missing, such as long chain fatty acid (LCFA) inhibition. The major variation in co-substrates composition poses a challenge for modelling AcoD since the model parameters have to be calibrated accordingly; and for dynamic simulations and evaluation of operational strategies, flexibility in feed composition is necessary since it also can vary over time. In the literature there are several examples of how to modify ADM1 for such purposes. The simplest approach is to characterise the actual feed mix. Derbal et al. (2009) uses the standard procedure from Batstone et al. (2002) to acquire the stoichiometric composition of composite particulate chemical oxygen demand (COD) (X_c), i.e. carbohydrates (X_{ch}), proteins (X_{pr}), lipids (X_{li}) and inerts (X_I). This approach is successful in terms of model predictions but leads to an inflexible model since the substrate mix cannot be varied without repeating the characterisation. Esposito et al. (2008) modelled AcoD of sewage sludge and food waste using a modified ADM1. For the degradation of particulate organic matter they used the standard formulation of ADM1 with disintegration and hydrolysis for all substrates and biomass decay. In order to separate the different streams they used multiple pools of composite material, i.e. X_{c1}, X_{c2}, etc. each with its individual disintegration kinetics. A more general and flexible method for