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Effects of ionic strength and ion pairing on (plant-wide) modelling of anaerobic digestion

Kimberly Solon [a], *Xavier Flores-Alsina* [b], *Christian Kazadi Mbamba* [c], *Eveline I.P. Volcke* [d], *Stephan Tait* [c], *Damien Batstone* [c], *Krist V. Gernaey* [b], *Ulf Jeppsson* [a,*]

[a] *Division of Industrial Electrical Engineering and Automation (IEA), Department of Biomedical Engineering, Lund University, Box 118, SE-221 00 Lund, Sweden*
[b] *CAPEC-PROCESS, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, DK-2800 Lyngby, Denmark*
[c] *Advanced Water Management Centre (AWMC), University of Queensland, St Lucia, Brisbane, Queensland 4072, Australia*
[d] *Department of Biosystems Engineering, Ghent University, Coupure Links 653, B-9000 Gent, Belgium*

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ABSTRACT

Plant-wide models of wastewater treatment (such as the Benchmark Simulation Model No. 2 or BSM2) are gaining popularity for use in holistic virtual studies of treatment plant control and operations. The objective of this study is to show the influence of ionic strength (as activity corrections) and ion pairing on modelling of anaerobic digestion processes in such plant-wide models of wastewater treatment. Using the BSM2 as a case study with a number of model variants and cationic load scenarios, this paper presents the effects of an improved physico-chemical description on model predictions and overall plant performance indicators, namely effluent quality index (*EQI*) and operational cost index (*OCI*). The acid-base equilibria implemented in the Anaerobic Digestion Model No. 1 (ADM1) are modified to account for non-ideal aqueous-phase chemistry. The model corrects for ionic strength via the Davies approach to consider chemical activities instead of molar concentrations. A speciation sub-routine based on a multi-dimensional Newton–Raphson (NR) iteration method is developed to address algebraic interdependencies. The model also includes ion pairs that play an important role in wastewater treatment. The paper describes: 1) how the anaerobic digester performance is affected by physico-chemical corrections; 2) the effect on pH and the anaerobic digestion products (CO_2, CH_4 and H_2); and, 3) how these variations are propagated from the sludge treatment to the water line. Results at high ionic strength demonstrate that corrections to account for non-ideal conditions lead to significant differences in predicted process performance (up to 18% for effluent quality and 7% for operational cost) but that for pH prediction, activity corrections are more important than ion pairing effects. Both are likely to be required when precipitation is to be modelled.

* *Corresponding author*. Tel.: +46 46 222 92 87; fax: +46 46 14 21 14.
E-mail address: ulf.jeppsson@iea.lth.se (U. Jeppsson).

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Nomenclature

γ	activity coefficient
ΔH^o	enthalpy change of the reaction
A_1, A_2, A_3	physico–chemical framework 1, 2 and 3
AD	anaerobic digestion
ADM1	Anaerobic Digestion Model No. 1
a_i or a_j	activity of the species (i) or component (j)
BSM2	Benchmark Simulation Model No. 2
COD	chemical oxygen demand
CSTR	continuous stirred tank reactor
DAE	differential algebraic equation
EQI	effluent quality index (kg pollution day^{-1})
Gas_{CH_4}	methane gas production (kg day^{-1})
Gas_{CO_2}	carbon dioxide gas production (kg day^{-1})
Gas_{H_2}	hydrogen gas production (kg day^{-1})
GISCOD	general integrated solid waste co-digestion
$G(Z_i)$	vector containing the values of the set of implicit algebraic equations ($g(z_1,\ldots,z_n)$, …, $g(z_1, \ldots,z_n)$)
I	ionic strength (mol L^{-1})
IWA	International Water Association
J_f	analytical Jacobian of first order partial derivatives $\delta(G_1, \ldots, G_m)/\delta(z_1, \ldots, z_n)$
K_i	equilibrium constant
N	nitrogen
N_C	number of components
NR	Newton–Raphson
N_{sp}	number of species
OCI	operational cost index
PCM	physico–chemical model
ODE	ordinary differential equation
R	universal gas constant (bar L mol^{-1} K^{-1})
S_{ac}	acetate concentration (kmol COD m^{-3})
S_{Al}	aluminium concentration (mol L^{-1})
S_{an}	anions concentration (mol L^{-1})
S_{bu}	butyrate concentration (kmol COD m^{-3})
S_{Ca^+}	calcium concentration (mol L^{-1})
S_{cat}	cations concentration (mol L^{-1})
S_{C_i}	ith scenario
S_{Cl}	Chloride concentration (mol L^{-1})
$S_{CO_3^{-2}}$	carbonate concentration (mol L^{-1})
S_{Fe}	iron concentration (mol L^{-1})
S_{H^+}	proton concentration (mol L^{-1})
$S_{H_2CO_3^*}$	carbonic acid concentration (mol L^{-1})
$S_{H_2PO_4^-}$	dihydrogen phosphate concentration (mol L^{-1})
S_{H_2S}	hydrogen sulfide concentration (mol L^{-1})
$S_{HCO_3^-}$	bicarbonate concentration (mol L^{-1})
$S_{HPO_4^{-2}}$	hydrogen phosphate concentration (mol L^{-1})
S_i	species concentration (mol L^{-1})
S_{IC}	inorganic carbon (kmol m^{-3})
S_{IN}	inorganic nitrogen (kmol m^{-3})
S_j	component concentration (mol L^{-1})
S_K	potassium concentration (mol L^{-1})
S_{Mg^+}	magnesium concentration (mol L^{-1})
S_{Na}	sodium concentration (mol L^{-1})
S_{NH_3}	ammonia concentration (mol L^{-1})
$S_{NH_4^+}$	ammonium concentration (mol L^{-1})
$S_{PO_4^{-3}}$	phosphate concentration (mol L^{-1})
S_{pro}	propionate concentration (kmol COD m^{-3})
$S_{SO_4^{-2}}$	sulphate concentration (mol L^{-1})
S_{va}	valerate concentration (kmol COD m^{-3})
T	temperature (K)
UASB	upflow anaerobic sludge blanket
WWTP	wastewater treatment plant
z_i	of ion i
Z_i	vector of equilibrium states ($z_{1,i}$, …, $z_{n,i}$)

1. Introduction

Anaerobic digestion is a proven waste stabilization technology which is widely applied and studied because of its beneficial production of renewable biogas energy, making it a truly sustainable technology. From a systems engineering point-of-view, one of the major advances in the field of anaerobic digestion has been the development of the International Water Association (IWA) Anaerobic Digestion Model No. 1 (ADM1) (Batstone et al., 2002). The ADM1 is a general structured model consisting of biochemical and physico-chemical processes, which is useful for the design, operation and optimization of anaerobic digestion plants (Batstone et al., 2006). The adoption of the ADM1 in popular systems analysis tools, such as the plant-wide benchmark simulation model for wastewater treatment plants (BSM2), and its use as a virtual industrial system can stimulate modelling of anaerobic processes by researchers and practitioners outside the core expertise of anaerobic processes (Jeppsson et al., 2013).

Anaerobic digestion models are still being extended to include: i) improved biodegradability predictions (Astals et al., 2013); ii) inhibition factors (Wilson et al., 2012; Zonta et al., 2013); and, iii) microbial diversity (Ramirez et al., 2009). The ADM1 has been successfully implemented into multiple tank configurations: continuous stirred tank reactors (CSTRs) (Rosen et al., 2006), upflow anaerobic sludge blanket (UASB) reactors (Batstone et al., 2005; Hinken et al., 2014) and biofilm reactors described by 1D (Batstone et al., 2004) and 2D/3D models (Picioreanu et al., 2005). Important aspects about modelling frameworks and methodologies for parameter estimation and model validation in the field of anaerobic digestion processes can be found in Donoso-Bravo et al. (2011). In addition to municipal wastewater treatment, other applications of the ADM1 have been hydrogen production (Penumathsa et al., 2008), blue-algae digestion (Yuan et al., 2014) or co-digestion processes using the general integrated solid waste co-digestion (GISCOD) model interface (Zaher et al., 2009). Along this line of thinking, the ADM1 could potentially be applied to the treatment of industrial waste, animal manure, landfill leachate and brine from reverse