Modelling and control in anaerobic digestion: achievements and challenges

D.J. Batstone

Advanced Water Management Centre, The University of Queensland; damienb@awmc.uq.edu.au

Abstract
Anaerobic digestion modelling has now reached a steady and broad application base, with publication of approximately 150 articles per year, of which approximately 50% reference the IWA ADM1. This paper reviews changes in application area, and finds that diversity of use has increased, with application by both specialist and non-specialist users, particularly for systems analysis, and identification of underlying process characteristics. However, the three areas of input/substrate characterisation, physicochemistry modelling, particularly in the plant wide context, and application of multidimensional modelling have been identified as key challenges. A systematic methodology for characterising diverse simple and complex substrates is a major barrier to model application. This has been addressed to a limited extent, focused on domestic streams, but needs to be developed further and generalised. Within physicochemistry, the need is broad, but requirements related specifically to plant wide domestic modelling of phosphorous are identified as relating to solid-liquid interactions and the sulfur cycle. This is critical to future phosphorous control and nutrient recovery. Multidimensional modelling is highly important to all areas of anaerobic process application, but barriers are mainly related to accessibility rather than technical issues, and in particular, broader application to solid phase digestion would be highly beneficial to optimisation of design and operation.

Keywords
Anaerobic Digestion Modelling; ADM1; review

INTRODUCTION

Tools, capability, perception, and application of anaerobic digestion modelling have shifted substantially since publication of the IWA Anaerobic Digestion Model No. 1 in 2002 (Batstone et al. 2002). Work around modelling of anaerobic digestion processes has now reached a steady reached a steady rate of approximately 150 publications per year, of which ½ are utilising or referencing directly the IWA ADM1 (approx. 750 citations since publication).

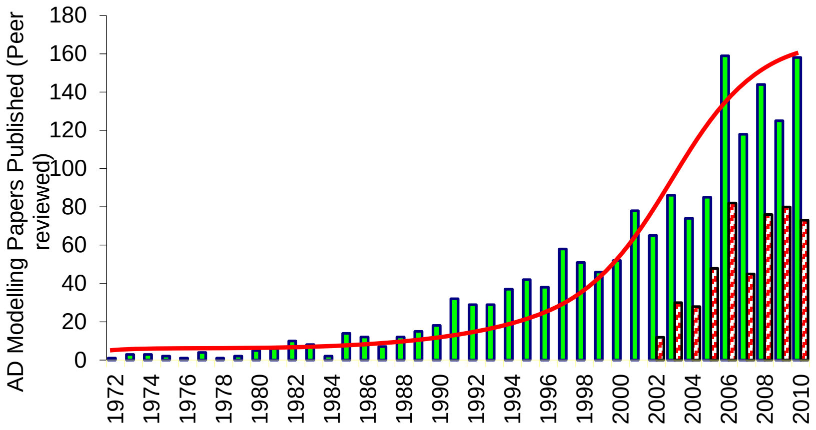

Figure 1: Papers with subject area anaerobic digestion modelling (solid) and subset citing ADM1 primary reference (shaded red).

However, this does not depict well changes in usage patterns. The last review of ADM1 developments and applications was done in 2005 (Batstone et al. 2006a) over 100 papers, and identified that a large proportion of papers had focused on initial application and parameter validation (Blumensaat and Keller 2005), particularly on implementation and testing of the base model (Rosen et al. 2006), as well as model extension to alternative materials such as sulfate, and potentially alternative bases (Fedorovich et al. 2003; Kleerebezem and van Loosdrecht 2006a). The base has certainly broadened substantially in the last 8 years, with key applications in the following areas (this is certainly not comprehensive):-

(a) Analysis of experiments, particularly identification of parameters and underlying characteristics of anaerobic systems (Donoso-Bravo et al. 2013; Ge et al. 2010)

(b) Its use as a generic tool to identify characteristics of a particular system (Pratt et al. 2012)

(c) Analysis of system fundamental characteristics, particularly in relation to other biological processes (Bernard et al. 2006; Grau et al. 2009)

(d) Use of anaerobic digestion models in either integrated system assessment, or for plant wide modelling, particularly greater use of dynamic integrated models (Corominas et al. 2012; Jeppsson et al. 2007)

(e) Its use in complex multidimensional systems (Batstone et al. 2006b)

This illustrates the far broader base of anaerobic digestion process modelling, and often application by non-anaerobic experts (for its application in integrated models), and its application for non-modelling experts (for its application in systems analysis). In particular, it has been used to identify the limits for control system application except in dynamic, highly loaded systems (Steyer et al. 2006). The rigorous approach being shown towards model application and identification is very encouraging (Batstone et al. 2009; Donoso-Bravo et al. 2011) which is now being applied to broader applications such as analysis of biochemical methane potential testing.

This broader application is of key importance given the future needs of anaerobic digestion modelling in the light of emerging needs such as nutrient recovery (Mehta and Batstone 2013), development of new processes such as thermophilic and ultra-high rate processes (Ge et al. 2011), and its application to tracking of micropollutants and recalcitrant (Fountoulakis et al. 2008). However, a number of deeper questions are emerging that are currently limiting application of anaerobic digestion modelling, and which potentially limit its usefulness in developing control systems. These largely relate to accessibility and applicability of the model, but also strongly apply to emerging systems as noted above. In particularly, three key topics have been nominated as challenges, due to their relevance to emerging processes or role in limiting uptake of digestion modelling. It should be noted that each of these topics has substantial enabling science, but that integrative steps need to be taken to realise application.

Key topics that are limiting application and which will be discussed further here include:-

(a) Input/substrate characterisation and translation.

(b) Physicochemical modelling (including solids precipitation), particularly with application to plant wide modelling and nutrient recovery.

(c) Multi-dimensional modelling.

INPUT/SUBSTRATE CHARACTERISATION AND TRANSLATION.

This is a problem across all anaerobic digestion modelling, not just application of the ADM1, and indeed, very substantial resources have been expended in characterising just the methane potential of a wide degree of materials for the simple purpose of estimating its methane potential in the environment (i.e. methane potential of wastes). This requires estimation of only chemical energy (i.e., COD), and degradability, but is known to vary substantially.

The challenge is larger for structured AD modelling, due to the following challenges:-

(a) Very important outputs such as pH and gas composition are inherently dependent on input carbon oxidation state.

(b) Different fractions are available that can degrade at different rates, or even interact (Mata-Alvarez et al. 2011)

(c) One needs to consider additional fractions that will contribute to the physicochemical system, including ammonia, buffering and potentially metals (Nopens et al. 2009)

The original ADM1 proposed for simple substrates and primary sludge to split to primary substrates (i.e., proteins, lipids, carbs, inerts), or for complex substrates such as activated sludge, to represent as complexes, X_c. Unfortunately, neither of these approaches works in practice, and the applying this approach can result in an unrealistic 2nd order process where both complexes and primary substrates have similar hydrolysis rates. In the first case, there are excessive degrees of freedom that can be solved stoichiometrically if degradability is known (Kleerebezem and Van Loosdrecht 2006b). However, it does not provide any assessment of the relative speeds of fractions. The second approach (i.e., X_c) does not account for changes in degradability or oxidation state with upstream plant operation (Gossett and Belser 1982).

Application in domestic applications has been partially addressed through an activated sludge interface model (Nopens et al. 2009), that is effective in characterising activated sludge, and there are developing characterisation rules based on batch tests (Girault et al. 2012), but there is no systematic approach. There is a need for a methodology that develops characterisation rules based on substrate type using either upstream knowledge (e.g., the Nopens model), chemical analysis (for simple substrates), or biochemical testing. This will be further evaluated in the presentation.

PHYSICOCHEMICAL MODELLING

The limitations of existing physicochemical models in the ASM1-3 and ADM1 have been extensively reviewed previously (Batstone et al. 2012). In particularly, different models are not state-compatible, do not describe precipitation (particularly of calcium and phosphate) across a variety of regimes, do not describe interactions at actual concentrations, and except for the ADM1, do not have pH as an output. This has been recognised as a problem in the past, particularly with respect to phosphorous modelling in anaerobic digesters and has been addressed with specific models (Sotemann et al. 2005). However, the problem needs a more comprehensive approach, with a major example being plant wide modelling of phosphorous. Specifically, phosphorous binds with iron in sewers and in aerobic processes, as iron sulfide is solubilised under sulfide oxidation. This is then released during anaerobic digestion due to binding of the iron with sulfide (generated from sulfate) (Ge et al. 2013). The released phosphorous then binds with calcium in the digester (an undesired process for nutrient recovery), and will bind with magnesium and ammonium downstream during potential recovery through struvite precipitation processes (a desired process) (Mehta and Batstone 2013). Calcium will then re-release during aerobic processes as iron sulfide solubilises and iron phosphate releases. This is obviously a complex cycle that is a ripe target for model based analysis, but requirements include:-

(a) A plant wide physicochemical model that adequately describes phosphate speciation and release under aerobic and anaerobic conditions. This needs to include multiple precipitation reactions and should be applicable across the range of environments being assessed.

(b) Inclusion of sulfur reduction and oxidation processes. This may require a suite of biological reactions that has the potential to double the size of the ADM1 (Fedorovich et al.

2003).

While complex, this offers very interesting potential for phosphorous control and recovery through manipulation of this cycle, which is only available if models exist. However, it offers very interesting potentials for phosphorous control and recovery through manipulation of this cycle, which is best addressed through mechanistic model based analysis. Addressing the problem in a systematic way would allow inclusion of a broad range of other processes, including nutrient recovery, and odour generation from secondary units. Identification of this challenge, as well as its opportunities in other areas of aquatic modelling have led to development of the IWA Taskgroup for Physicochemical modelling, which is focused on generalised modelling of physicochemical processes.

MULTIDIMENSIONAL MODELLING

Unlike the other two challenges identified here, multidimensional modelling does not require codification, development, and validation of new concepts. Indeed, it has been well established and applied to anaerobic digestion modelling (Batstone et al. 2006b; Vavilin et al. 2002). However, accessibility is limiting its necessary application to a broad range of processes. Almost any process being analysed within the range of anaerobic digestion processes has variation in space as well as time. At the same time, analysis of anaerobic digestion systems is almost uniformly based on fully mixed assumptions, or at best, using tank-in-series approximations. Taking common systems:-

(a) Sludge digesters are frequently limited by mixing. The interaction between mixing and performance has been only evaluated in a limited way (Wu 2012).

(b) Large scale systems such as lagoons can be strongly limited by solids accumulation and degradation.

(c) High-rate anaerobic systems such as UASB and IC/EGSB reactors can be dominated by hydraulic characteristics but are generally modelled using CSTR kinetics (Batstone et al. 2005). The influence of hydraulics will become increasingly important as application of high-rate anaerobic digestion, including emerging systems such as Anaerobic MBR systems are increasingly applied to low strength wastes such as domestic wastewater.

(d) In particular, there has been very limited application of anaerobic modelling to solid phase and semi-solid plug flow systems (Fezzani and Ben Cheikh 2008). This is a major limitation, particularly as these systems can be strongly optimised in terms of design and operation by model-based analysis.

The fact that significant work has been done demonstrates the potential to apply AD modelling in these environments (particularly computing speed is now adequate), but the problem mainly relates to accessibility and approach, which will be further discussed in the presentation.

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