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REVIEW PAPER

Mathematical modelling of anaerobic digestion processes: applications and future needs

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Abstract Anaerobic process modelling is a mature and well-established field, largely guided by a mechanistic model structure that is defined by our understanding of underlying processes. This led to publication of the IWA ADM1, and strong supporting, analytical, and extension research in the 15 years since its publication. However, the field is rapidly expanding, in terms of new technology, new processes, and the need to consider anaerobic processes in a much broader context of the wastewater cycle as a whole. Within the area of technologies, new processes are emerging (including high-solids and domestic wastewater treatment). Challenges relating to these new processes, as well as the need to intensify and better operate existing processes have increased the need to consider spatial variance, and improve characterisation of inputs. Emerging microbial processes are challenging our understanding of the role of the central carbon catabolic metabolism in anaerobic digestion, with an increased importance of phosphorous, sulfur, and metals as electron source and sink, and consideration of hydrogen and methane as potential electron sources. The paradigm of anaerobic digestion is challenged by anoxygenic phototrophism, where energy is relatively cheap, but electron transfer is expensive. These new processes are commonly not compatible with the existing structure of anaerobic digestion models. These core issues extend to application of anaerobic digestion in domestic plant-wide modelling, with the need for improved characterisation, new technologies having an increased impact, and a key role for the linked phosphorous–sulfur–iron processes across the cycle. The review overall finds that anaerobic modelling is increasing in complexity and demands on the modeller, but the core principles of biochemical and physicochemical processes, metabolic conservation, and mechanistic understanding will serve well to address the new challenges.

Keywords ADM1 · AnMBR · Leach bed · Plug-flow · Hydraulics · Phosphorous · Iron · Sulfur

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1 Introduction

Probably the most common technical question since publication of the IWA Anaerobic Digestion Model No. 1 (Batstone et al. 2002) has been "When will the ADM2 be published?". Indeed, it was asked during presentation of the ADM1 in Brussels in 2010 at AD IX. At that time, it was due to apprehension that the model would be replaced in 1–2 years, but since then (and in the 13 years since publication), there has been genuine interest as to what should replace, eventually, the ADM1.

So far, there has been no compelling reason to release an ADM2 as such. The ADM1 itself was based on a broad range of other, largely comparable models (Angelidaki et al. 1999; Costello et al. 1991b; Kalyuzhnyi and Fedorovich 1998a; Siegrist et al. 1993; Vavilin et al. 1997), which did not vary substantially in concept, only implementation. Its strengths were broad basis and concept compatibility with the IWA ASM series (Henze et al. 2000), a clear and complete presentation of all model elements, as well as reference implementations, and importantly (given the large numbers of parameters), a complete and consistent parameter set. However, given the amount of previous model development work, it is unlikely that model structure would change substantially, unless core alternative processes (e.g., acetate oxidation) were found to have (Wett et al. 2014) a far higher incidence than thought, or to be inadequately described by extensions, there is no current need for a re-release of the core model. Indeed, the main (structural) part of the ADM1 which was original, has caused some problems, and is input of complex particulates as X_c, which is undefined and generally causes continuity issues when coupled to other models (Nopens et al. 2009). This is discussed further in Sect. 4.

While there is limited need for changes in biochemical structure (and this need can be largely addressed by plugins), or the underlying COD-uptake-yield structure (note there has been some discussion of this (Kleerebezem and van Loosdrecht 2006), a number of limitations have emerged, particularly over the last 5 years, which the aggregate modelling literature is not addressing sufficiently, or in a sufficiently comprehensive way. This review focuses on identifying and discussing these fairly disparate issues, and proposes initial approaches to address them. Scope is limited to mechanistic and semi-mechanistic models, with stochastic models (e.g. García-Gen et al. 2015; Pullammanappallil et al. 1998) including multi-order empirical, regressive, and expert systems models forming another class of models, with generally a focus on system characterisation for control and soft sensors, and system optimisation, rather than understanding and fundamental characterisation as is used in mechanistic models.

2 New technologies

The last 10 years have seen substantial expansions in the range of technologies utilised in anaerobic digestion. This is further reviewed recently (Batstone and Rodriguez 2015; Batstone and Virdis 2014; Jensen et al. 2014b), but broaden the scope of anaerobic technologies to new applications. These utilise improved understanding of the underlying process, and its kinetic or metabolic limitations [e.g., plug-flow anaerobic digestion (Dvorak 2012)], or advances in associated wastewater treatment technologies such as aerobic membrane bioreactor processes to enable high-solids wastewater treatment through anaerobic membrane bioreactors (Liao et al. 2006). A summary is shown in Fig. 1. This shows historic processes such as mixed digesters and traditional high-rate processes (UASB reactors, internal circulation, EGSB), as well as anaerobic lagoons and waste stabilisation lagoons, which remain very common for tropical and subtropical (and even temperate) climates (Shilton and Harrison 2003).

Modelling goals are also shown in Fig. 1, with those around historic processes being relatively mature, and focused on specific problems, and those around emerging processes focused on elementary process description.

2.1 Anaerobic lagoons/waste stabilisation ponds

Anaerobic lagoons are generally deeper and often used for primary wastewater treatment (Shilton and Harrison 2003) and industrial wastewater treatment (Jensen et al. 2014b). Key operational problems are hydraulic design (Shilton and Harrison 2003), including the response of hydraulics to changes in ambient temperature, and accumulation of solids, also

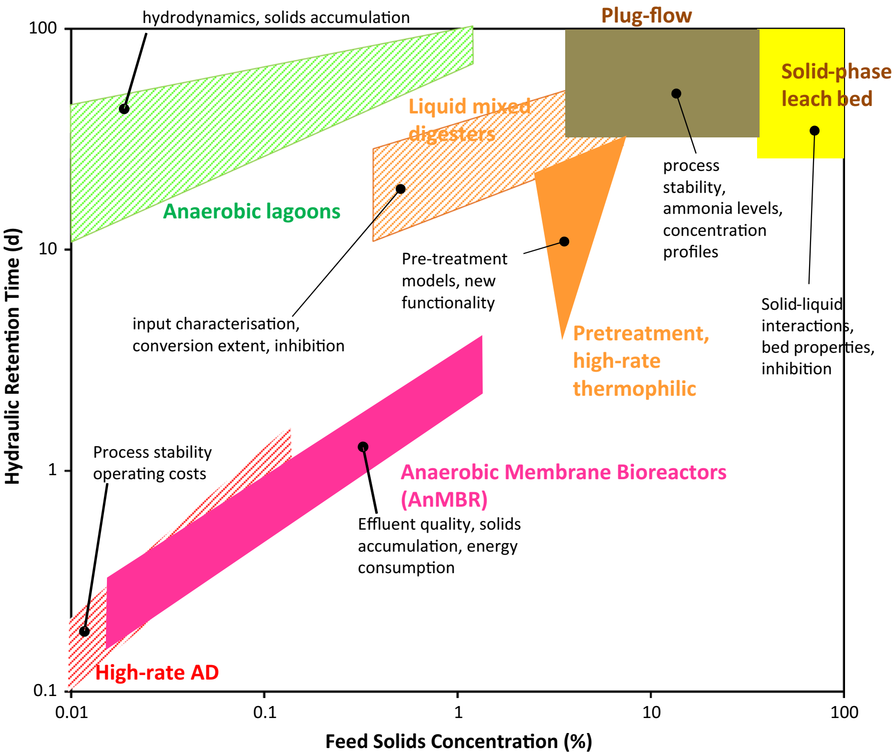

Fig. 1 Emerging processes in Anaerobic Digestion (shown in *solids fill*) against hatched existing processes). Key modelling goals and needs are also shown

including the effect of temperature (Papadopoulos et al. 2003).

Non-biological, hydraulic modelling only has been extensively used to address the issue of hydraulic design (see review in Shilton and Harrison 2003), but these have not generally been combined with biological models, mainly due to numerical complexity and model stability when coupling biological rate equations with CFD equations. Simplified hybrid models have been used (Alvarado et al. 2012), as a stirred-tank hydraulic combined with biological kinetics would be inappropriate given the complex hydraulics.

So far the problem of sludge accumulation has been addressed only through simple stirred tank or compartmentalised reaction (1st order) accumulation models (Saqqar and Pescod 1995).

The two problems of sludge accumulation and hydraulics are complex and linked. As lagoons are covered to capture methane, costs of desludging and methane loss will increase, which increases the motivation to model. At the same time, the ability to simultaneously model hydraulics, biological transformations, and distributed behaviour of sludge (as well as sludge-hydraulic coupling) will continue to improve by the use of reactive CFD. The difficulty has been noted above, but this is quite realisable given current techniques, and hence represents an opportunity. This is a primary example of a problem where multi-phase reactive distributed parameter modelling is core to the overall problem.

2.2 Liquid mixed digesters

Anaerobic sludge digestion was original focus of kinetic modelling of anaerobic processes (Gossett and Belser 1982; Pavlostathis and Gossett 1986) as well as a key focus for the ADM1 and similar models (Batstone et al. 2002; Siegrist et al. 2002). This is hence one of the most mature applications of anaerobic process modelling, and remains a key focus.

The key challenge in this area is that of input characterisation (kinetics and stoichiometry), as principal issue in system and parameter identification, especially with particulate substrates where hydrolysis coefficient, energy density, and degradable fraction define performance under the majority of operating states (Donoso-Bravo et al. 2011; Jensen et al. 2011). Due to fundamental limitations, the complex particulate concept (X_c) in the ADM1, or analogous states in other models (Siegrist et al. 2002) has been generally discarded (see discussion in Sect. 4), and inputs defined as inerts (X_I), and degradable, either aggregate, or separated into carbohydrates, lipids, and proteins (the latter approach enables energy density and nitrogen fraction to be defined).

Approaches to characterisation have either been biological, using a batch test or on-line data to enable estimation of parameters (Batstone et al. 2009; Girault et al. 2012; Jensen et al. 2011), direct chemical measurement, either inferential (e.g., COD, N, VS), or directly (Buffiere et al. 2008; Zaher et al. 2009), or by empirical techniques (e.g., spectroscopy and correlation analysis) (Jimenez et al. 2014). Another approach is upstream model based analysis (or continuity based on whole plant modelling (De Gracia et al. 2011; Nopens et al. 2009). This is a highly active area that is only now seeing some consolidation into a defined approach, and a key issue is translation and comparison between different approaches, as well as validation in full-scale systems, with, often kinetics being difficult to estimate (Jensen et al. 2011).

Another emerging focus in mixed-digester modelling has been the emergence of mixed feed digestion (Mata-Alvarez et al. 2011), and codigestion with sewage sludges, particularly of opportunistic feeds such as glycerol (Jensen et al. 2014a) and fats, oils, and greases (FOG) (Razaviarani and Buchanan 2015). The use of modelling to enable mechanistic analysis of mixed feed digestion is particularly important (Astals et al. 2014), potentially to identify the underlying basis for synergistic (Pagés-Díaz et al. 2015), or antagonistic (Long et al. 2012) responses. Many of the underlying mechanisms are well represented in structured models such as the ADM1, which particularly include the balance between pH depression caused by increased carbohydrate degradation, and elevation (and potential ammonia inhibition) caused by increased protein degradation. Mechanisms such as LCFA and glycerol inhibition may need to be added, and there is some evidence that threshold style rather than non-competitive is a more appropriate function, even for biostatic inhibitors such as ammonia, salts, and organic acids (Astals et al. 2015; Pratt et al. 2012). Physicochemical and hence pH modelling is undergoing revision, including complex chemistry, precipitation, and the linked phosphorous-sulfur cycles, and this is discussed further in Sects. 3 and 4.

Computational fluid dynamics has been widely used to evaluate digester mixing efficiency, but distributed parameter models are now being coupled to reactive models such as the ADM1 (Gaden 2014; Van Hulle et al. 2014), mainly to investigate the impact of non-ideal mixing on process performance.

Other emerging areas of anaerobic modelling mainly related to the increased use of pretreatment to enhance degradability speed and extent. To date, this has mainly focused on characterising the effect of enhancement [reviewed extensively in (Carrère et al. 2010)], but there is further work identifying how new pathways such as acetate oxidation (Rivera-Salvador et al. 2014; Wett et al. 2014) may influence response from pretreatment, or play a role in high-rate, high temperature anaerobic digestion (Ho et al. 2014).

2.3 Biofilm high-rate anaerobic digestion

This analysis focuses on biofilm high-rate anaerobic digestion, which includes biofilters and granular high-rate systems, including upflow anaerobic sludge blanket (UASB), attached film fixed and fluidized bed, expanded granular sludge bed (EGSB), and internal circulation reactors (IC). It should be noted that granular systems from a biofilm modelling perspective are simply self supporting biofilms, and approaches are generally common. These systems have an extensive history of modelling, mainly focused on process modelling, particularly process modelling of the balance between acid producing and acid consuming processes (Costello et al. 1991a), but also (for example), competition for electrons (Kalyuzhnyi and Fedorovich 1998a). A further review of classic anaerobic biofilm process modelling (granular and non-granular) is provided in (Saravanan and Sreekrishnan 2006). There has been more recent work in combined hydraulic-reactive modelling, for example, particularly novel reactor designs such as the spiral granular process (Chen et al. 2012), but also in conventional granular systems (Batstone et al. 2005), expanding from 1-D to multidimensional (Ren et al. 2009). Consideration of degradable substrate as media (a shrinking core combined with growing biofilm) expands application to solids substrates (see Sect. 2.6; da Rocha et al. 2013). Another historic focus has been modelling biofilm structure [reviewed in (Saravanan and Sreekrishnan 2006)], with this extending to multidimensional analysis to evaluate the microscopic effects of interspecies (Batstone et al. 2006). An emerging field has been on modelling new applications for this technology, with a key application being domestic wastewater treatment. This requires effective description of low-temperature operation (Donoso-Bravo et al. 2013), inclusion of sulfate as an electron acceptor, and inclusion of methane solubility (Batstone 2006). This has now translated particularly to application of emerging high-rate processes.

2.4 Emerging non-biofilm High-Rate (ABR, AnMBR)

Anaerobic baffled reactors (ABR) have been extensively used as an alternative to biofilm systems, particularly for low strength wastewater (Barber and Stuckey 1999), and this analysis has extended to model based analysis, both of hydrodynamics, and kinetics [see recent review (Zhu et al. 2015)]. ABRs are particularly interesting where each stage is measured, as kinetics are exposed by the relatively short hydraulics in the first stage, which enables effective parameter identification.

However, the major development in high-rate systems over the last 5 years has been widespread application of anaerobic membrane bioreactor (AnMBR) systems, particularly for domestic wastewaters. This is now a very large field, and full coverage is beyond the scope of this review, a number of reviews have been done, all of which highlight low-strength wastewater treatment, including applications (Liao et al. 2006), issues (particularly technical extensions) (Stuckey 2012) as well as a review specifically on domestic wastewaters (Ozgun et al. 2013). These together provide an excellent review of the scope, applications, and issues in anaerobic MBR systems, which commonly are flux management, dissolved methane control, optimal design and configuration, and generation of byproducts and behaviour of recalcitrant components. They also highlight the advantages of AnMBR systems, which are inherent decoupling of hydraulic and solids retention times, production of high-quality effluent, ever-decreasing energy consumption (Shin et al. 2014), and the ability to apply to a broad range of novel processes (Batstone and Virdis 2014). Evolution of AnMBR designs have been evident, towards the now dominant design of hollow fibre submerged AnMBR systems.

The reviews have not extensively assessed modelling of AnMBRs, but it is an active area, with a current focus that aligns with the outcomes of the reviews above. The strongest focus of modelling has been on fouling prediction and control, with particularly the work of Robles addressing this problem in developing a mechanistic cake accumulation model (Robles et al. 2013b) and applying both mechanistic and empirical models for cake accumulation control (Robles et al. 2013a, 2014). Cake accumulation models have also been combined with CFD in a multi-dimensional domain (Boyle-Gotla et al. 2014). However, these have not generally considered biological reactions. Reactive models have been applied to general AnMBR issues, considering accumulation of soluble inerts (Benyahia et al. 2013), general performance modelling (Spagni et al. 2015). However, what has not been done is reactive modelling to link accumulation and presence of particular constituents such as colloidal organics, fats, and SMP, as well particulate and reactive membrane cakes to fouling (Dereli et al. 2015).

There is clearly strong scope for increased coupling of reactive process modelling and reactor design, with a particular focus on coupling hydraulics, membrane physical interactions, and multiphase reactions to further optimise this promising process.

2.5 Plug flow reactors (PFR)

Plug glow reactors are increasingly being used, particularly in North America for high-solids manure digestion system. Plug flow anaerobic digestion feeds sludge at a high concentration (8–12 %) with the solids moving progressively along a rectangular or circular cross-section trench and reducing to 3–6 % at the outlet. Hydraulic retention time is normally >20 days, but space use is effective due to high solids concentration and the enhanced kinetics of plug flow digesters. The very high ammonia concentrations (3–5 gN L^{-1}) enabled by high feeds solids provide inherent protection against low pH failure, such that the key consequence is an elevated organic acid level (>1000 mg COD L^{-1}). There is very limited formal literature on plug flow reactors, with some found on microbial community (Li et al. 2014). Designs can be relatively simple, or more complex and engineered e.g., the DVO design has a sophisticated U-shaped digester design, with gas induced corkscrew mixing, ammonia recovery by pH and temperature elevation (to 70 °C), and use of high-pH effluent to scrub gas of CO_2 and H_2S (with the gas being used to reduce effluent pH due to supply of CO_2 as an acid) (Frear and Dvorak 2013). Ammonia stripping is enabled by high temperature and high pH applied during ammonia stripping by DVO.

Plug flow reactors are subject to an interesting set of process constraints. The hydraulics allow better utilisation of the volume, but increases risk of overloads, where less effective buffering is provided by the digester volume. Put simply, if the digester fails near the start, that failure can progressively spread to the remainder of the digester. However, the very high ammonia concentrations (3–5 gN L^{-1}) enabled by high feeds solids provide inherent protection against low pH failure, such that the key consequence is an elevated organic acid level (>1000 mg COD L^{-1}). This is a problem that can be addressed readily through anaerobic process modelling and dominant mechanisms of convection-reaction. Designs also utilise potentially gas lift radial mixing, which could benefit from CFD (or coupled CFD-kinetics).

2.6 Leach bed reactors (LBR)

Leach bed reactors (LBRs) apply a reactive percolation liquid to digest a solid phase at high concentrations. The liquid can be simply recirculated, or further treated through a high-rate anaerobic process (e.g., biofilter (Linke et al. 2015)), or chemical process such as ammonia removal. The leach bed is most commonly operated in batch or semi-batch mode (Gehring et al. 2015), but continuous mode operation is also possible (Linke et al. 2015). LBRs have been widely applied to grass, straw, and maize silage (Gehring et al. 2015; Linke et al. 2015), municipal solid bioreactors (la Cour Jansen 2011), animal manures (Saritpongteeraka et al. 2014), and is generally applicable to any structured solid substrate. They are also applicable to generation of alternative products such as hydrogen and organic acids (Lei et al. 2015).

Leach bed systems are complex to operate, with the feeds being largely carbohydrates (i.e., poorly buffered), often having high ammonia levels from the outset, and existing in multi-stage configuration with mixed batch-continuous processes. They generally do not achieve the full methane potential of the underlying substrates (Lei et al. 2015).

Fundamentally, LBRs are also one of the most complex systems to simulate effectively, containing gas, liquid and reactive solid phases, as well as complex interactions between biologically active solids and liquid and gas flows (q_L, q_G in Fig. 2). Particularly as a batch process, the hydraulics and effective volume of the solid bed can change, which then has an integrated impact on concentration in the liquid phase. An outline of the interacting processes is shown in Fig. 2. Modelling is limited, and approaches can be divided into those that apply a lumped parameter approach to identify process characteristics (Nopharatana et al. 2003), and those that attempt to represent the full mechanistic process. The latter are impressive, and generally develop strong insight into how these fundamentals interact. ADM1-style models have been applied, including simulation of the high-rate leachate treatment process (e.g., (Thamsiriroj et al. 2012), CFD and changes in bed porosity have been considered (Shewani et al. 2015). Municipal landfills represent a large scale leachbed, with modelling largely focused on the water balance (Berger et al. 1996), since this predicts leachate generation, but also with some process modelling (Kim et al. 2007). However, with the emergence of engineered landfills and in-vessel municipal digestion (Chugh et al. 1999),

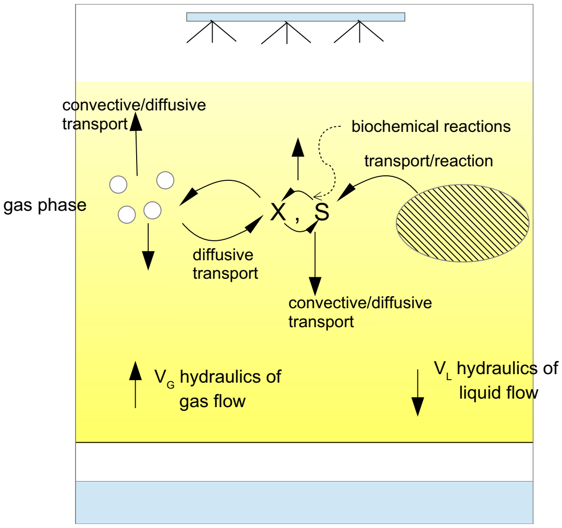

Fig. 2 Mechanisms for modelling in a leach bed system, including mass transport, and multi-phase reaction between particulate phase (X) and the soluble phase (S) [modified from (Batstone and Rodriguez 2015)]

this will be an increased target for mechanistic modelling.

One of the reasons that mechanistic modelling is useful is that leach bed reactors fully expose potential imbalances between acid producing processes and acid consuming, as these are generally separated between the bed and the high-rate reactor, and this requires a mechanistic modelling approach. The balance of factors can vary substantially between crop residues (which are carbohydrate dominated, and represent souring behaviour), and manures and municipal solids waste, which have higher ammonia levels, and hence can be dominated by ammonia inhibition. Particularly coupling dynamic long-term changes in bed physical characteristics with mass transport, reaction, and the relatively short term changes that occur in the high-rate anaerobic reactor is a challenging problem that offers the potential for insight into how to optimise these processes towards the performance of mixed digesters.

2.7 Conclusions: technologies

Anaerobic modelling has now evolved to the point where evaluation of existing processes, as well as the requirements of new reactors is exposing the limits of treating the digester as a completely mixed process. This is most evident in emerging processes such as leach bed reactors and plug-flow reactors. However, it is also becoming more important in systems such as sludge digesters, high-rate anaerobic systems, and anaerobic MBRs, where aggregate performance can be adequately simulated by a mixed tank, but challenging situations such as high-solids, co-feeds, or membrane-fluid coupling require consideration of spatial variance. This is increasing the importance of including spatial variance (including potentially coupling CFD and reactive models), and techniques are either developing, or on the cusp of being available to properly consider and apply modelling to achieve fundamental insight into- and improvements that would not otherwise be enabled. We also note that anaerobic processes are not limited to engineered systems, and in fact, the principles of anaerobic modelling can be applied to the natural environment (with soil and marine methane cycles being critical—see Sect. 3 discussing environmental anaerobic cycles). Another fascinating (and advanced application) is simulation of gut processes, from a basic analytical perspective (Muñoz-Tamayo et al. 2010), but also from an advanced perspective, using mechanistic modelling to determination variation in both processes and physical configuration (Godon et al. 2013), which can provide clues as to how to potentially build a better anaerobic digester.

3 Emerging anaerobic processes

Anaerobic digestion modelling has been extensively applied to investigate the core processes themselves (nominally those that appear in the ADM1), but also a variety of alternative organic substrates such as lactate (Hinken et al. 2014) and ethanol (Peiris et al. 2006). Alternative electron acceptors are another key topic (see below). However, modelling problems associated with novel processes are now emerging that need a rethink as to what constitutes an "anaerobic" process.

The classical scheme of the anaerobic digestion pathway should be particularly transformed into another concept where the major electron flows from inorganic sources would be depicted. Figure 3 shows a mechanistic scheme of the anaerobic transformations occurring in a digester where the emerging anaerobic processes are included. A summary of key aspects of these emerging processes is reviewed in Table 1.

3.1 Electrons without organics: chemo and lithotrophic processes (nitrogen, sulfur, metals, and hydrogen)

3.1.1 Anaerobic nitrogen conversions

Anaerobic digestion is characterised by a lack of electron acceptors, such that the substrate itself becomes the terminal electron acceptor. In practice, this occurs by the major intermediates carbon-dioxide (CO_2) and hydrogen (H_2), such that excess electrons are used (via H_2) to reduce carbon-dioxide to methane. This has been extensively discussed in the ADM1 report (Batstone et al. 2002) and elsewhere, and hydrogen transfer to methanogens is energetically and diffusively limited, and one of the governing mechanisms in anaerobic processes. Anaerobic processes are inherently electron-rich, and hence alternative, more favourable electron acceptor molecules are readily utilised. The key alternative electron acceptors are sulfate and nitrate/nitrite.

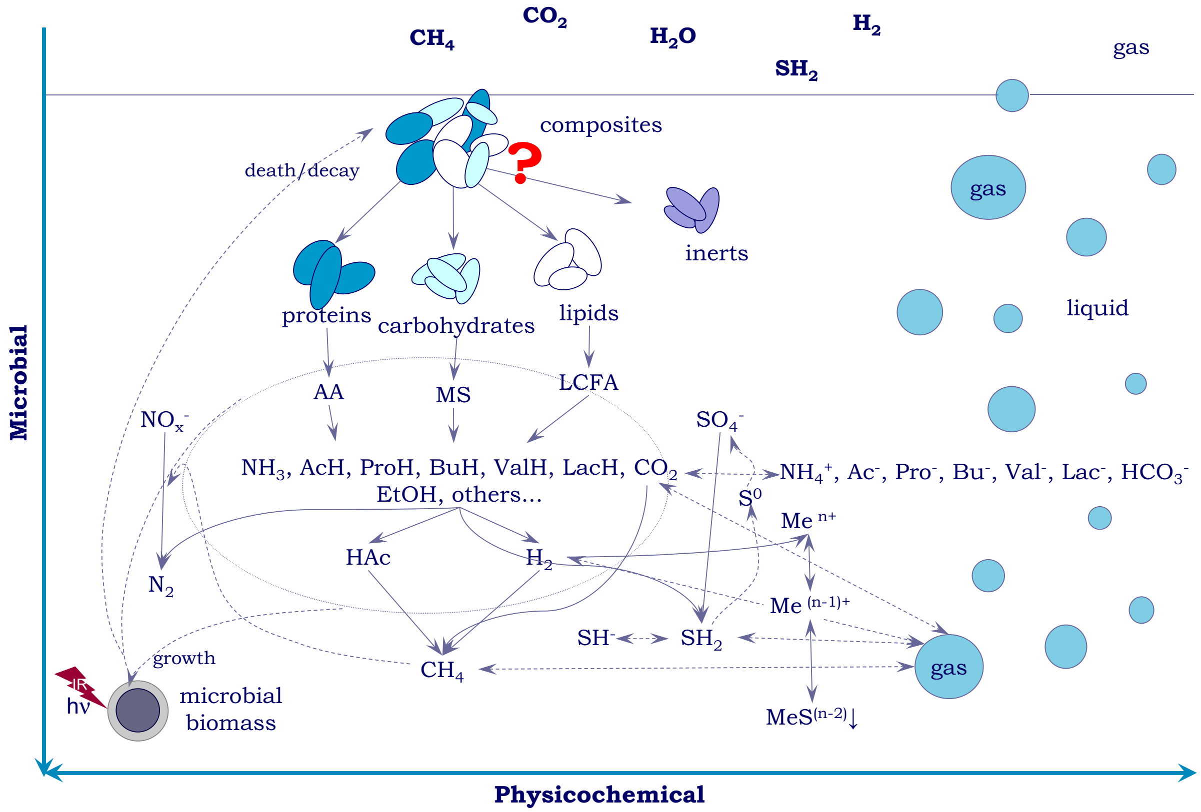

Fig. 3 Emerging metabolic processes in anaerobic digestion, including photo-anaerobic processes, sulfur-cycle (which interacts with the phosphorous cycle), metal oxidation–reduction cycles, alternative nitrogen cycles, and the action of methane and hydrogen as electron donor. The ADM1 representation of composites is shown as contested (?) due to issues raised in Sect. 4

Both inhibition and utilisation of nitrate in general anaerobic digester conditions has been comprehensively assessed (Tugtas et al. 2010), and oxidised forms of nitrogen are short-lived in the aggregate digester. However, more complex problems are now emerging. Methane has generally been regarded as inert under anaerobic conditions, but is known to be (slowly) reactive under aerobic condition (Lieberman and Rosenzweig 2004). The focus for this has been biomanufacturing of polymers using methane as substrate. However, oxidised nitrogen has also been found to act as electron acceptors for the anoxic oxidation of methane (denitrifying anaerobic methane oxidation, DAMO process) (Raghoebarsing et al. 2006). This is further complicated by the fact that two domains respectively reduce nitrate to nitrite (archaea) and nitrite to nitrogen gas (bacteria) (Chen et al. 2014). The process is obviously of interest in wastewater treatment due to the ability to use methane to denitrify, and nitrate/nitrite to remove methane from mainline anaerobic treatment (McCarty et al. 2011). A simple model has been proposed that encompasses the two DAMO processes as a sole mechanisms and also includes substrate inhibition by nitrite (He et al. 2013). Another model encompases archeal DAMO only but also incorporates alternative electron acceptors such as Fe^{3+}, Mn^{4+} or SO_4^{2-}. The model is geochemically-oriented but the mechanisms are similar to those appearing in DAMO reactors. It does not include inhibition processes (Lopes et al. 2011), which are very important for the nitrite producing archaeal DAMO. A challenge in investigating this are that the organisms are extremely slow growing, and in fact, the bacteria can be outcompeted for nitrite by anammox organisms (Chen et al. 2014), a mechanism which has been considered in the Chen model (Chen et al. 2014). Modelling the complex interaction between DAMO and anammox organisms

Table 1 Key catabolic mechanisms of emerging anaerobic processes

Process	Key catabolic equation	Modeling challenges
Anaerobic ammonium oxidation	$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O$	Complex substrate inhibition Catabolism uncoupled to anabolism
Denitrifying anaerobic methane oxidation	$CH_4 + 4NO_3^- \rightarrow CO_2 + 4NO_2^- + 2H_2O$ $3CH_4 + 8NO_2^- + 8H^+ \rightarrow 3CO_2 + 4N_2 + 10\ H_2O$	Very slow growth rate requires almost perfect biomass retention Two-domain model with archaea utilizing nitrate
Sulfide oxidation	$HS^- + 2O_2 \rightarrow SO_4^{2-} + H^+$ $HS^- + H^+ + \frac{1}{2} O_2 \rightarrow S^0 + H_2O$	Two-step process mediated by oxygen concentration
Sulfate reduction (H_2 only shown)	$4H_2 + SO_4^{2-} + H^+ \rightarrow HS^- + 4\ H_2O$	Competition with acetogens and methanogens Sulfide production can bind metals
Photoheterotrophic uptake[a]	$C_4H_6O_4 + 2NAD^- + Light \rightarrow 2NADH + H^+ + C_4H_4O_4$	Very complex metabolism Competence and mutualism with other microorganisms makes models complex
Anoxygenic photosynthesis[a]	$H_2 + NAD^- + Light \rightarrow NADH + H^+$	Light harvesting makes the models highly complex High nutrient uptake make uses highly dependent on growth

[a] Other substrates and electron donors are omitted for the sake of simplicity. Metals oxidation/reduction not included

is important, since denitrifying archaea can coexist with either DAMO bacteria or anammox, but the latter two compete for nitrite.

Another key anaerobic N process is the anaerobic ammonium oxidation (Anammox). Modelling of Anammox in general is undergoing challenge and revision. A suitable model for Anammox conversions was published early (Koch et al. 2000), and has been widely applied. However, the catabolism is complex due to physical and inorganic interactions and the complex internal organization of the anammox cell. Additional inhibitory factors include the effect of pH, especially in underload situations(Carvajal-Arroyo et al. 2014a), and inhibition due to both unionized acids (free nitrous acid –FNA– and free ammonia –FA–) as well as ionized nitrite, which has an acute inhibitory effect on anammox activity (Puyol et al. 2014). Added to this is the ability of the organisms to store polymers (van Niftrik et al. 2008a), and maintenance requirements in challenging conditions (Carvajal-Arroyo et al. 2014a, b). Metallic interactions have also been found, with Fe(III) deposits accumulating in the anammoxosome complex (van Niftrik et al. 2008b), which may be a product of reduction reactions, or possibly related to FNA oxidation to form free radicals that help explain the role of FNA.

Overall, the anaerobic nitrogen cycle is complex, involving multiple competing organisms mediating multiple processes, and important, in both anaerobic and anoxic environments. This area requires more work, particularly in consolidation and analysis of mixed population systems.

3.1.2 Anaerobic sulfur conversions

Anaerobic sulfur cycling includes both sulfate reduction to sulfide, as well as potentially sulfide oxidation to both elemental sulfur and sulfate due to nitrate and fugitive (or intentionally) added oxygen or air. It is metabolically diverse, and connected to carbon, phosphorous, and even Fe and As cycles (Rodriguez-Freire et al. 2014) in anaerobic, and general wastewater treatment (see Sect. 4).

The classical key process in the sulfur cycle is the biological sulfate reduction performed by sulfate reducing bacteria (SRB) (Hao et al. 2014). These chemotrophic bacteria are able to anaerobically reduce the sulfate both autolithotrophically (using H_2 as e-donor and CO_2 as C source) and heterorganotrophically (using organic compounds as e-donor and C source). Sulfate reduction was not incorporated in the original ADM1 but it is relatively easy to implement as a side or main process (Fedorovich et al. 2003). SRB generally outcompete acetogens for organic substrate and with hydrogenotrophic methanogens for hydrogen (Kalyuzhnyi and Fedorovich 1998b). The produced sulfide is inhibitory (Utgikar et al. 2002). Strategies for inclusion are either to only include competition for hydrogen (Batstone 2006), or to include also competition with acetogens (Kalyuzhnyi and Fedorovich 1998b). The latter substantially increases model complexity efforts. Where the influent sulfate:COD ratio is relatively low, a reduced model (Batstone 2006) offers a fair representation of the S transformation processes. At high sulfate levels, it is possible that hydrogen is depleted and SRB use organic acids as source of electrons, and the sulfate reduction model should be upgraded with these additional biochemical routes (Barrera et al. 2015) (see also Barrera et al. 2013). Sulfate reduction is being increasingly assessed in metal sulfide interactions, and as a potential platform for metals recovery (Weijma et al. 2002). Relevant metals are $Fe^{2+,3+}$, Zn^{2+}, Cu^{2+}, Pb^{2+}, Cr^{2+}, Ni^{2+} or Cd^{2+} with particular application to mining wastewater flows (Tang et al. 2009). Apart from metal partitioning, there are also biological effects in reduction of metals toxicity (Gonzalez-Estrella et al. 2015), and metabolic interactions (Bridge et al. 1999).

Sulfide oxidation through microaerobic treatment is a low cost method to remove sulfides through addition of small amounts of air or oxygen into gas or liquid phases (Diaz and Fdz-Polanco 2012; Jenicek et al. 2008). When sulfide is oxidised in a digester at limited oxygen levels, it reacts to elemental sulfur (requiring only 0.5 mol O_2 per mole S^{2-}). Availability is then limited for further biological reduction, which means air injection is effective for sulfide control. A new recent process has been discovered relating the sulfur cycle with the phosphorous cycle which is particularly interesting in enhanced biological phosphorus removal (EBPR) processes (Wu et al. 2013). This process leads to recover S as S^0 globules production in a syntrophic association between EBPR and S-cycle bacteria, theoretically allowing to recovery also P as Poly-P and C as PHA and to eliminate N in a nitrification/autotrophic denitrification step (Wu et al. 2014). This process has been recently proposed and still needs more confirmation about the complete biological mechanisms, so there is a clear opportunity associated to the development of a model to describe accurately this complex bacterial association.

3.1.3 *Other metallotrophic and lithotrophic processes*

While many metallotrophic processes involve the sulfur cycle [that of arsenic being particularly fascinating (Rodriguez-Freire et al. 2014)], there are many examples of direct metal reduction, including of naturally iron (Lovley et al. 1987) but also exotics such as uranium (Lovley et al. 1991) and chromium (Focardi et al. 2013) as covered in the biogeochemical literature. This is also important to processes such as anaerobic biocorrosion, with sulfate reducers known to directly accept electrons from metallic iron surfaces (Chen et al. 2015), and the produced hydrogen sulfide acting as electrochemical catalyst (Enning and Garrelfs 2014). Paradoxically, the mechanism of iron sulfide precipitation attenuates, rather than accelerates corrosion due to the loss of the catalyst. Modelling metal-microbe interactions, particulary in the wastewater sector is limited, given its importance on the phosphorous and sulfur cycles.

The other important non-carbon emerging substrate is hydrogen. Hydrogen as an alternative product to methane (via particularly fermentation) has historically been a research target, including detailed modelling (Penumathsa et al. 2008). In particular, variable stoichiometry fermentation models have been a strongly researched field (González-Cabaleiro et al. 2015), with broader applicability to biotechnology and understanding of microbial metabolism and electron management (Hoelzle et al. 2014). However, a new focus for hydrogen is emerging with the increasing need to store peak electricity from renewables, and the ease of generating hydrogen electrochemically, and need to upgrade methane for vehicle and grid use, hydrogen to methane is now of interest. This has been shown to be relatively simple, with digesters generally having excess capacity and fast response to hydrogen addition (Díaz et al. 2015; Zhang et al. 2013). The key issues are availability of bicarbonate and managing pH. While references to modelling this have not been found, the ADM1 in stock form is capable of modelling the bulk processes and controlling mechanisms. Electrogenic methane production in the reactor on carbon cathodes is also of interest (Cheng et al. 2009) (though configuration is a challenge), and there is still debate as to whether this occurs via cathodic hydrogen production (enhanced by biological catalysts), or by direct electron transfer. The basic principles of electron addition (via hydrogen or other) can of course be extended to VFA synthesis (Zhang et al. 2013), which requires exclusion of archaea but is an important area for the emerging biorefinery field.

3.2 Energy without electrons: anoxygenic phototrophic bacteria (purple phototrophic bacteria)

The use of biological light-consuming processes for wastewater treatment is not new (Munoz and Guieysse 2006) with a focus on algae and photosynthetic bacteria (which reduce CO_2 to organics producing oxygen as electron sink). However, non-photosynthetic treatment has been promoted in recent years driven by the extraordinary and complex metabolism of phototrophic bacteria, which are among the most metabolically diverse organisms existing (Hunter 2008). They also mediate biogeochemical cycles of C, N, P, S, H and Fe (Hunter 2008). Recently, purple phototrophic bacteria (PPB) have been proposed as an alternative to aerobic waste activate sludge (WAS) processes in mainline domestic wastewater treatment via assimilative, rather than reactive carbon and nitrogen removal (Batstone et al. 2015), with complete, single step domestic wastewater treatment demonstrated in principle (Hülsen et al. 2014). This adds to research on the use of PPB for treating industrial wastewater in pure (Kim et al. 2004) and mixed culture (Chitapornpan et al. 2013) systems. One of the important aspects of PPB is the ability to operate without sterile systems due to use of infrared light, which enables PPB to outcompete other heterotrophic and methanogenic organisms (Hülsen et al. 2014).

Because PPB grow anoxygenically there is an excess of electrons to dispose, but they only can sink electrons via biosynthesys or, alternatively, by hydrogen production via the nitrogenase complex (Fang et al. 2005), and hence the COD (electron) balance between catabolism and anabolism is almost 1 (McKinlay and Harwood 2010). Since they are phototrophic but also chemotrophic, fermentative and anaerobic oxidation mechanisms can be applied to model their metabolism. But the most important mechanism of PPB is photoheterotrophy (Gordon and McKinlay 2014; McKinlay and Harwood 2010), which involves the coupling of the TCA and Calvin-Benson cycles with an ETC fuelled by light energy in a cyclic electron re-use (anoxygenic cyclic phosphorylation). PPB cannot source electrons from water (photosynthetic organisms) but can oxidise reduced compounds such as Fe^{2+}, HS^{-}/S^{2-}, $S_2O_3^{-}$ or H_2 (Overmann and Garcia-Pichel 1998). Further complicating this, PPB bacteria can storage poly-P as well as carbon PHA and polysaccharides (Brandl et al. 1991; Klein et al. 1991; Liang et al. 2010; Melnicki et al. 2009). However, unlike other polymer and poly-P organisms, energy for accumulation is derived from light, which means they can store under anaerobic conditions. This means that the ASM2d (Henze et al. 2000) is not applicable to PPB.

Metabolic models have been developed for PPB oriented to explain the complex metabolism of these bacteria (Golomysova et al. 2010; Klamt et al. 2002) but these are unsuitable for wastewater applications. Such a model needs inclusion of photoheterotrophy on different substrates, photoautotrophy by using hydrogen, chemotrophy of simple organics with concomitant hydrogen production, and also incorporate hydrolysis of particulates and biomass decay. Other potential mechanisms include, especially for polyphosphate accumulation, potentially nitrogen fixation where this is limiting, and engagement in the sulfur cycle. This is clearly a challenge for which existing modelling paradigms are unsuitable.

3.3 Conclusions: processes

We now need to expand substantially our understanding of what constitutes an “anaerobic” process, with new processes not focused on the core carbon metabolism, and emergence of anaerobic processes (such as phototrophic growth), where energy, translated directly to ATP is cheap, but electron transfer is expensive. While most of these processes are not catered for by the existing structure of anaerobic digestion models, the core principles of biochemical and physicochemical processes, metabolic conservation, and mechanistic understanding are applicable, and the same approach used to analyse these exciting new processes.

4 Whole wastewater treatment plant modelling

Plant-wide modelling of wastewater treatment has been a key focus particularly in development of commercial software (for example, Biowin is inherently a plant-wide model, while other packages enable plant-wide modelling), and this includes modelling of the sludge digester, as not only does generation of methane and digestion of solids influence operating costs, but performance also influences the rest of the plant through release of nitrogen and phosphorous in the reject water. The goal of integrating the ADM1 within plant wide modelling was done very early by the benchmarking taskgroup (Rosen et al. 2006), and this development (and further development) have highlighted a number of compatibility issues between the ASM series (Henze et al. 2000) and the ADM1, and some core limitations of the IWA models in general. The Benchmark Simulation Model No. 2 has recently been released (Gernaey et al. 2014), and contains plant wide nitrogen and carbon cycle simulation, but not phosphorous. This section reviews needs for plant wide modelling (one of the key focuses for anaerobic process modelling), in conjunction with other needs identified above.

4.1 Input translation: the problem with X_c

When different models with different states are linked, a translator is needed that preserves state continuity between the different models. That is, translates ASM states such as X_S, S_S etc. to ADM1 states such as X_{ch}, S_{su}, S_{ac}. This translator should also ensure elemental continuity (CHONSP) and maintain a consistent physicochemical state, even though acids and bases may be removed or transformed through the interface (i.e., pH). The alternative is plant wide state continuity through a common model such as used in the ASDM in Biowin (see also Grau et al. 2009).

Development of the interface within the BSM2 identified that the complex organics state (X_c) was unsuitable as a primary input (which was its intended purpose), due to a number of reasons, including:

(a) Fixing of nitrogen content, and carbon oxidation state, and degradability (to the underlying value of X_c), without the ability to readily and separably vary for primary and activated sludge. This also has the potential to violate continuity in a plant wide model.

(b) Implementation of the two step process of disintegration followed by hydrolysis means that the overall solubilisation process becomes two-step, in opposition to evidence (Batstone et al. 2009; Vavilin et al. 1996). This can be artificially addressed by artificially raising the hydrolysis rate (or disintegration rate), but is an otherwise unnecessary circumvention and unmechanistic. It also results in artefacts around anaerobic decay.

It is therefore ironic that the X_c state is somewhat unsuitable for use in its primary purpose to characterise wastewater sludges. For the reasons above, the BSM2 interface model used carbohydrates, proteins, and lipids as primary input (Nopens et al. 2009), and we also recommend this approach in general (i.e., substrates in general should be characterised on this basis using the methodologies outlined in Sect. 2.2.

4.2 Phosphorous modelling

Plant wide phosphorous modelling has been a challenge in general, and particularly where different models are used for activated sludge and anaerobic digestion processes. Only the group at University of Cape Town (Ekama et al. 2006) has addressed the problem in a plant wide context. Phosphorous modelling is however, an essential requirement of future models, particularly considering the focus on phosphorous load in many catchments, need to recovery phosphorous, and its new transformations in emerging processes (Batstone et al. 2015). It is noted that this is not just a problem relating to activated sludge BNR processes, but also all emerging processes identified in Sect. 2, particularly high-strength, domestic, or manure, and links into many of the new processes identified in Sect. 3.

Considering plant wide modelling, both ASM (specifically the ASM2d for phosphorous) and ADM1 models are inadequate to consider plant wide modelling. Part of this is because the physicochemistry models in both do not consider more complex effects such as ion activity and ion pairing, which strongly influence phosphate availability, and hence its partitioning in precipitates (Batstone et al. 2012). Indeed, plant-wide P description requires continuous ionic strength tracking; extensive consideration of non-ideality (including ion activities instead of molar concentrations) and consideration of complexation processes (Flores-Alsina et al. 2015). The other issue is additional biological transformation of phosphorous (see Sect. 4.2.2 for details). Finally, as outlined in S3.1.1 and S4.2.3 there is a strong interaction with the sulphur and iron cycle. Hence both physicochemical and biological process extensions are needed in a plant wide context. A summary of the processes is included in Fig. 4.

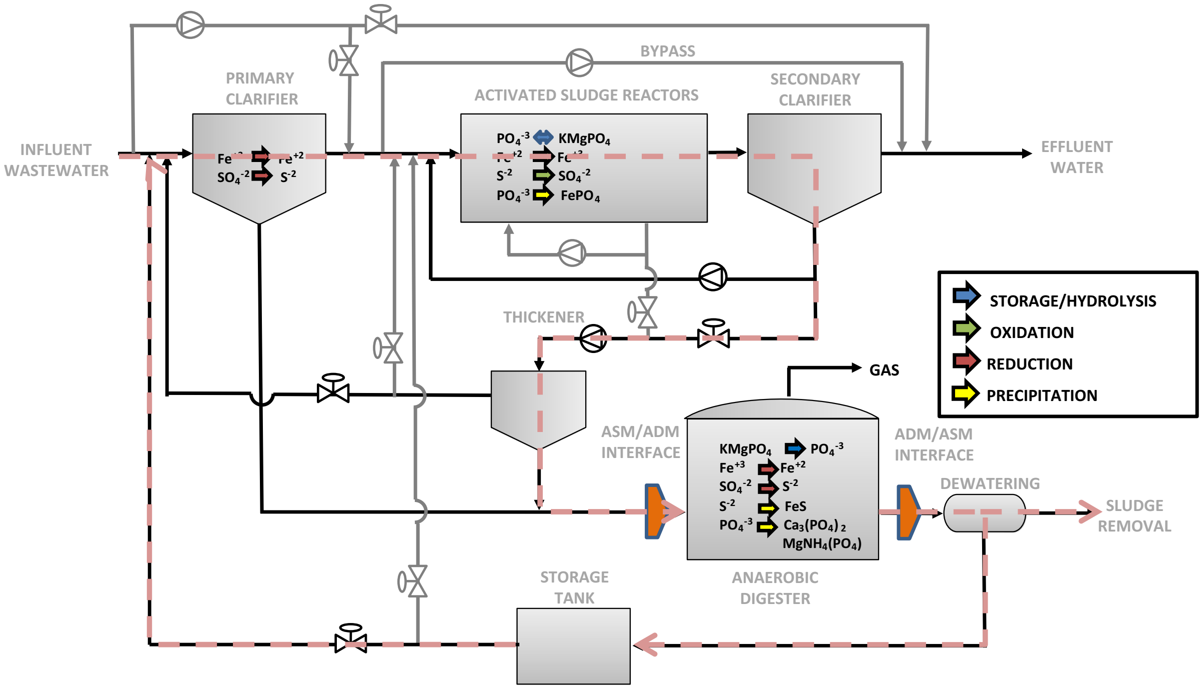

Fig. 4 Plant wide P transformations, including flow of phosphorous in the system

4.2.1 *ASM/ADM interface*

The first interface between ASM and ADM is based on the methodology described in Nopens et al. (2009). When including P and a plant wide physicochemical approach (see Sect. 4.2.2), this approach should further expanded with the Continuity-Based Model Interfacing principle (CBIM) (Volcke et al. 2006) ensuring elemental conservation principles. It is important to highlight that depending how P is modelled in the AD, Phosphorus Accumulating Organisms (PAOs), poly-hydroxy-alkanoates (PHA) and poly-phosphates (PP) will be treated differently. Methods may include instantaneous decay and translation in the interface, or dynamically (via uptake/decay processes) within the AD model. In any case, the total COD, C, N, P, S, K, Mg, Fe… load would at both sides of the interface will be the same, but the distribution amongst the different state variables will be different.

4.2.2 *Physicochemical*

The physicochemical problem is readily addressed by implementation of a plant-wide common physicochemical model, which also addresses the interface problem. This is justified on the basis that acid–base active components (particularly elemental ions) are generally present throughout the process, and that reasonable and consistent plant-wide pH prediction is a core requirement. The case for a generalized plant-wide pH model has been extensively made previously (Batstone et al. 2012), and resulted in formation of the IWA Taskgroup for a Generalized Physicochemical Model (PCM). Taskgroup activities have resulted in proposals for implementation of pH (including activity and ion speciation/pairing) in the ASM/ADM series (Flores-Alsina et al. 2015; Solon et al. 2015), generalized precipitation using this model (Kazadi Mbamba et al. 2015a, b), and application of a generalized physicochemical approach including precipitation (Lizarralde et al. 2015) in the plant wide biological model of Grau et al. (2007).

4.2.3 *Biological*

The ASM2d effectively considers the role PAOs in the line (Henze et al. 2000). Similar processes should be included in the sludge line (Ikumi et al. 2011) describing the effect that PAOs, PHA, PP might have on the anaerobic digestion products (biogas, phosphorus precipitates). However, these models do not consider the interaction with sulfur and iron under aerobic or anaerobic conditions. This metal-phosphorous-sulfur interaction is complex, and affects the whole water cycle (Pikaar et al. 2014). In brief, sulfate is reduced to sulfide in the sewer and primaries, with the sulfide binding with $Fe^{2/3+}$, which causes phosphorous to release. The sulfide is biologically reoxidised to sulfur and sulfate in the activated sludge process, and iron oxidised to Fe^{3+}. This releases iron to bind with phosphorous (iron phosphate), at the same time as biological assimilation and poly-P (PP) accumulation occurs. In the anaerobic digester, sulfate is again reduced to sulfide. Both precipitated (iron phosphate) and biological phosphorous (PP, biomass) might be chemically and biologically released through both re-dissolution of iron phosphate and hydrolysis of PP (Ge et al. 2013). Because of a pH increase, calcium and magnesium phosphates are formed/precipitated. At the same time, Fe^{3+} is reduced to Fe^{2+} (using hydrogen or sulphide as electron donors). The latter can precipitate in form of FeS reducing the overall sulfide inhibition of the AD bacteria and potential corrosion/odour problems. Some of these processes have been discussed in Sect. 3, and require a considerable extension to the base models, depending on (for example) the complexity of the phosphorus/sulphur/iron model used.

4.3 Conclusion on whole wastewater treatment plant models

Plant wide P modelling has a profound impact, particularly at physico-chemical level. As a key wastewater treatment objective, it will require a major, but unavoidable, additional degree of complexity when representing cationic/anionic behaviour in activated sludge (AS)/anaerobic digestion (AD) models. An important factor to consider is the close interaction between the S and the Fe system. Therefore, reliable P plant wide model predictions should also consider including these elements (Se, Fe) when describing the fate of the different pollutant at plant wide level.

5 Conclusions

The consistent themes throughout this review are increased demands on modelling, in terms of complexity, particularly in anabolic processes, need to consider complex behaviour (including distributed parameter and non-linear characteristics in space), and the need to better characterise inputs and their primary conversion processes, as well as supporting models such as the chemistry models. There are commonalities between the challenges in all three areas examined, particularly the emerging importance of non-carbon metabolisms (especially sulfur), and its interactions with other cycles, including that of the iron and phosphorous cycles. While the problems have increased in complexity, the approaches used so far are highly compatible with these new challenges, and application of the existing methodologies will enable a consistent and transparent approach. As to the original question: Is an ADM2 required? It is evident that modelling is currently being used in a productive way to support science and engineering, but the models being used are still in a state of flux. While there are readily justifiable and uniform modifications (such as removal of the X_c state), to move forward with a common basis for an ADM2, a uniform approach to the many challenges and mechanisms is needed, which may require still further development of the underlying research.

References

Alvarado A, Vedantam S, Goethals P, Nopens I (2012) A compartmental model to describe hydraulics in a full-scale waste stabilization pond Water Research 46:521–530. doi:10.1016/j.watres.2011.11.038

Angelidaki I, Ellegaard L, Ahring BK (1999) A comprehensive model of anaerobic bioconversion of complex substrates to biogas Biotech Bioeng 63:363–372

Astals S, Batstone DJ, Mata-Alvarez J, Jensen PD (2014) Identification of synergistic impacts during anaerobic co-digestion of organic wastes. Bioresour Technol 169:421–427

Astals S, Batstone DJ, Tait S, Jensen PD (2015) Development and validation of a rapid test for anaerobic inhibition and toxicity. Water Res 81:208–215. doi:10.1016/j.watres.2015.05.063

Barber WP, Stuckey DC (1999) The use of the anaerobic baffled reactor (ABR) for wastewater treatment: a review. Water Res 33:1559–1578. doi:10.1016/S0043-1354(98)00371-6

Barrera EL, Spanjers H, Dewulf J, Romero O, Rosa E (2013) The sulfur chain in biogas production from sulfate-rich liquid substrates: a review on dynamic modeling with vinasse as model substrate. J Chem Technol Biotechnol 88:1405–1420. doi:10.1002/jctb.4071

Barrera EL, Spanjers H, Solon K, Amerlinck Y, Nopens I, Dewulf J (2015) Modeling the anaerobic digestion of canemolasses vinasse: extension of the Anaerobic Digestion Model No. 1 (ADM1) with sulfate reduction for a very high strength and sulfate rich wastewater. Water Res 71:42–54. doi:10.1016/j.watres.2014.12.026

Batstone DJ et al (2002) Anaerobic Digestion Model No. 1 (ADM1), IWA task group for mathematical modelling of anaerobic digestion processes. IWA Scientific and Technical Reports. IWA Publishing, London

Batstone DJ (2006) Mathematical modelling of anaerobic reactors treating domestic wastewater: rational criteria for model use. Rev Environ Sci Biotechnol 5:57–71. doi:10.1007/s11157-005-7191-z

Batstone DJ, Rodriguez J (2015) Chapter 7: modelling anaerobic digestion processes. In: Fang HPP, Zhang T (eds) Anaerobic biotechnology: environmental protection and resource recovery. Imperial College Press, Singapore

Batstone DJ, Virdis B (2014) The role of anaerobic digestion in the emerging energy economy. Curr Opin Biotechnol 27:142–149. doi:10.1016/j.copbio.2014.01.013

Batstone DJ, Hernandez JLA, Schmidt JE (2005) Hydraulics of laboratory and full-scale upflow anaerobic sludge blanket (UASB) reactors. Biotechnol Bioeng 91:387–391. doi:10.1002/bit.20483

Batstone DJ, Picioreanu C, van Loosdrecht MCM (2006) Multidimensional modelling to investigate interspecies hydrogen transfer in anaerobic biofilms. Water Res 40:3099–3108. doi:10.1016/j.watres.2006.06.014

Batstone DJ, Tait S, Starrenburg D (2009) Estimation of hydrolysis parameters in full-scale anerobic digesters. Biotechnol Bioeng 102:1513–1520

Batstone DJ et al (2012) Towards a generalized physicochemical framework. Water Sci Technol 66:1147–1161. doi:10.2166/wst.2012.300

Batstone DJ, Hülsen T, Mehta CM, Keller J (2015) Platforms for energy and nutrient recovery from domestic wastewater: a review. Chemosphere 140:2–11. doi:10.1016/j.chemosphere.2014.10.021

Benyahia B, Sari T, Cherki B, Harmand J (2013) Anaerobic membrane bioreactor modeling in the presence of soluble microbial products (SMP): the Anaerobic Model AM2b. Chem Eng J 228:1011–1022. doi:10.1016/j.cej.2013.05.073

Berger K, Melchior S, Miehlich G (1996) Suitability of hydrologic evaluation of landfill performance (HELP) model of the US Environmental Protection Agency for the simulation of the water balance of landfill cover systems. Environ Geol 28:181–189. doi:10.1007/s002540050092

Boyle-Gotla A, Jensen PD, Yap SD, Pidou M, Wang Y, Batstone DJ (2014) Dynamic multidimensional modelling of submerged membrane bioreactor fouling. J Membr Sci 467:153–161. doi:10.1016/j.memsci.2014.05.028

Brandl H, Gross RA, Lenz RW, Lloyd R, Fuller RC (1991) The accumulation of poly(3-hydroxyalkanoates) in Rhodobacter sphaeroides. Arch Microbiol 155:337–340

Bridge TA, White C, Gadd GM (1999) Extracellular metal-binding activity of the sulphate-reducing bacterium Desulfococcus multivorans. Microbiology 145(Pt 10): 2987–2995

Buffiere P, Frederic S, Marty B, Delgenes JP (2008) A comprehensive method for organic matter characterization in solid wastes in view of assessing their anaerobic biodegradability, 58. doi:10.2166/wst.2008.517

Carrère H, Dumas C, Battimelli A, Batstone DJ, Delgenès JP, Steyer JP, Ferrer I (2010) Pretreatment methods to improve sludge anaerobic degradability: a review. J Hazard Mater 183:1–15

Carvajal-Arroyo JM, Puyol D, Li G, Sierra-Álvarez R, Field JA (2014a) The role of pH on the resistance of resting- and active anammox bacteria to NO_2—inhibition. Biotechnol Bioeng 111:1949–1956. doi:10.1002/bit.25269

Carvajal-Arroyo JM, Puyol D, Li G, Swartwout A, Sierra-Álvarez R, Field JA (2014b) Starved anammox cells are less resistant to inhibition. Water Res 65:170–176. doi:10.1016/j.watres.2014.07.023

Chen XG, Zheng P, Qaisar M, Tang CJ (2012) Dynamic behavior and concentration distribution of granular sludge in a super-high-rate spiral anaerobic bioreactor. Bioresour Technol 111:134–140. doi:10.1016/j.biortech.2012.02.044

Chen X, Guo J, Shi Y, Hu S, Yuan Z, Ni B-J (2014) Modeling of simultaneous anaerobic methane and ammonium oxidation in a membrane biofilm reactor. Environ Sci Technol 48:9540–9547. doi:10.1021/es502608s

Chen Y, Tang Q, Senko JM, Zhang Newby B-M, Castaneda H, Ju L-K, Cheng G (2015) Long-term survival of Desulfovibrio vulgaris on carbon steel and associated pitting corrosion. Corros Sci 90:89–100. doi:10.1016/j.corsci.2014.09.016

Cheng S, Xing D, Call DF, Logan BE (2009) Direct biological conversion of electrical current into methane by electromethanogenesis. Environ Sci Technol 43:3953–3958. doi:10.1021/es803531g

Chitapornpan S, Chiemchaisri C, Chiemchaisri W, Honda R, Yamamoto K (2013) Organic carbon recovery and photosynthetic bacteria population in an anaerobic membrane photo-bioreactor treating food processing wastewater. Bioresour Technol 141:65–74. doi:10.1016/j.biortech.2013.02.048

Chugh S, Chynoweth DP, Clarke W, Pullammanappallil P, Rudolph V (1999) Degradation of unsorted municipal solid waste by a leach-bed process. Bioresour Technol 69:103–115. doi:10.1016/S0960-8524(98)00182-5

Costello DJ, Greenfield PF, Lee PL (1991a) Dynamic modelling of a single-stage high-rate anaerobic reactor-I. Model Deriv Water Res 25:847–858. doi:10.1016/0043-1354(91)90166-N

Costello DJ, Greenfield PF, Lee PL (1991b) Dynamic modelling of a single-stage high-rate anaerobic reactor -I. Model Dev Wat Res 25:859–871

da Rocha D, Paetzold E, Kanswohl N (2013) The shrinking core model applied on anaerobic digestion. Chem Eng Process 70:294–300. doi:10.1016/j.cep.2013.05.003

De Gracia M, Huete E, Beltrán S, Grau P, Ayesa E (2011) Automatic characterisation of primary, secondary and mixed sludge inflow in terms of the mathematical generalised sludge digester model. Water Sci Technol 64:557–567. doi:10.2166/wst.2011.541

Dereli RK, Heffernan B, Grelot A, van der Zee FP, van Lier JB (2015) Influence of high lipid containing wastewater on filtration performance and fouling in AnMBRs operated at different solids retention times. Sep Purif Technol 139:43–52. doi:10.1016/j.seppur.2014.10.029

Diaz I, Fdz-Polanco M (2012) Robustness of the microaerobic removal of hydrogen sulfide from biogas. Water Sci Tech 65:1368–1374. doi:10.2166/wst.2012.013

Díaz I, Pérez C, Alfaro N, Fdz-Polanco F (2015) A feasibility study on the bioconversion of CO2 and H2 to biomethane by gas sparging through polymeric membranes. Bioresour Technol 185:246–253. doi:10.1016/j.biortech.2015.02.114

Donoso-Bravo A, Mailier J, Martin C, Rodríguez J, Aceves-Lara CA, Wouwer AV (2011) Model selection, identification and validation in anaerobic digestion: a review. Water Res 45:5347–5364

Donoso-Bravo A, Bandara WMKRTW, Satoh H, Ruiz-Filippi G (2013) Explicit temperature-based model for anaerobic digestion: application in domestic wastewater treatment in a UASB reactor. Bioresour Technol 133:437–442. doi:10.1016/j.biortech.2013.01.174

Dvorak SW (2012) Biosolids digester and process for biosolids production. PCT/US2010/058012

Ekama GA, Wentzel MC, Loewenthal RE (2006) Integrated chemical-physical processes kinetic modelling of multiple mineral precipitation problems, 53. doi:10.2166/wst.2006.407

Enning D, Garrelfs J (2014) Corrosion of iron by sulfate-reducing bacteria: new views of an old problem. Appl Environ Microbiol 80:1226–1236. doi:10.1128/aem.02848-13

Fang HHP, Liu H, Zhang T (2005) Phototrophic hydrogen production from acetate and butyrate in wastewater. Int J Hydrogen Energy 30:785–793. doi:10.1016/j.ijhydene.2004.12.010

Fedorovich V, Lens P, Kalyuzhnyi S (2003) Extension of anaerobic digestion model no. 1 with processes of sulfate reduction. Appl Biochem Biotechnol Part A Enzyme Eng Biotechnol 109:33–45

Flores-Alsina X, Kazadi-Mbamba C, Solon K, Vrecko D, Tait S, Batstone D, Jeppsson U, Gernaey KV (2015) A plant-wide aqueous phase chemistry module describing pH variations and ion speciation/pairing in wastewater treatment process models. Water res. doi: 10.1016/j.watres.2015.07.014

Focardi S, Pepi M, Focardi SE (2013) Microbial reduction of hexavalent chromium as a mechanism of detoxification and possible bioremediation applications. In: Chamy R (ed) Biodegradation life of science. pp 321–348. doi:10.5772/56365

Frear C, Dvorak S (2013) Commercial demonstration of nutrient recovery of ammonium sulfate and phosphorus rich fines from AD effluent

Gaden D (2014) Modelling anaerobic digesters in three dimensions: integration of biochemistry with computational fluid dynamics. University of Manitoba, Manitoba

García-Gen S, Rodríguez J, Lema JM (2015) Control strategy for maximum anaerobic co-digestion performance. Water Res 80:209–216. doi:10.1016/j.watres.2015.05.029

Ge H, Zhang L, Batstone D, Keller J, Yuan Z (2013) Impact of iron salt dosage to sewers on downstream anaerobic sludge digesters: sulfide control and methane production. J Environ Eng 139:594–601. doi:10.1061/(ASCE)EE.1943-7870.0000650

Gehring T et al (2015) Determination of methanogenic pathways through carbon isotope (δ13C) analysis for the two-stage anaerobic digestion of high-solids substrates. Environ Sci Technol 49:4705–4714. doi:10.1021/es505665z

Gernaey KV, Jeppsson U, Vanrolleghem PA, Copp JB (2014) Benchmarking of control strategies for wastewater treatment plants. IWA Publishing, London

Girault R et al (2012) A waste characterisation procedure for ADM1 implementation based on degradation kinetics. Water Res 46:4099–4110. doi:10.1016/j.watres.2012.04.028

Godon J-J, Arcemisbéhère L, Escudié R, Harmand J, Miambi E, Steyer J-P (2013) Overview of the oldest existing set of substrate-optimized anaerobic processes: digestive tracts. Bioenerg Res 6:1063–1081. doi:10.1007/s12155-013-9339-y

Golomysova A, Gomelsky M, Ivanov PS (2010) Flux balance analysis of photoheterotrophic growth of purple nonsulfur bacteria relevant to biohydrogen production. Int J Hydrogen Energy 35:12751–12760. doi:10.1016/j.ijhydene.2010.08.133

González-Cabaleiro R, Lema JM, Rodríguez J (2015) Metabolic energy-based modelling explains product yielding in anaerobic mixed culture fermentations. PLoS ONE. doi:10.1371/journal.pone.0126739

Gonzalez-Estrella J, Puyol D, Sierra-Alvarez R, Field JA (2015) Role of biogenic sulfide in attenuating zinc oxide and copper nanoparticle toxicity to acetoclastic methanogenesis. J Hazard Mater 283:755–763. doi:10.1016/j.jhazmat.2014.10.030

Gordon GC, McKinlay JB (2014) Calvin cycle mutants of photoheterotrophic purple nonsulfur bacteria fail to grow due to an electron imbalance rather than toxic metabolite accumulation. J Bacteriol 196:1231–1237. doi:10.1128/JB.01299-13

Gossett JM, Belser RL (1982) Anaerobic digestion of waste activated sludge. J Environ Eng ASCE 108:1101–1120

Grau P, de Gracia M, Vanrolleghem PA, Ayesa E (2007) A new plant-wide modelling methodology for WWTPs. Water Research 41:4357–4372. doi:10.1016/j.watres.2007.06.019

Grau P, Copp J, Vanrolleghem PA, Takács I, Ayesa E (2009) A comparative analysis of different approaches for integrated WWTP modelling. Water Sci Technol 59:141–147

Hao TW et al (2014) A review of biological sulfate conversions in wastewater treatment. Water Res 65:1–21. doi:10.1016/j.watres.2014.06.043

He Z, Cai C, Geng S, Lou L, Xu X, Zheng P, Hu B (2013) Modeling a nitrite-dependent anaerobic methane oxidation process: parameters identification and model evaluation. Bioresour Technol 147:315–320. doi:10.1016/j.biortech.2013.08.001

Henze M, Gujer W, Mino T, van Loosdrecht M (2000) Activated sludge models ASM1, ASM2, ASM2d, and ASM3. IWA Scientific and Technical Report, London

Hinken L, Huber M, Weichgrebe D, Rosenwinkel KH (2014) Modified ADM1 for modelling an UASB reactor laboratory plant treating starch wastewater and synthetic substrate load tests. Water Res 64:82–93. doi:10.1016/j.watres.2014.06.044

Ho D, Jensen P, Batstone D (2014) Effects of temperature and hydraulic retention time on acetotrophic pathways and performance in high-rate sludge digestion. Environ Sci Technol 48:6468–6476

Hoelzle RD, Virdis B, Batstone DJ (2014) Regulation mechanisms in mixed and pure culture microbial fermentation. Biotechnol Bioeng 111:2139–2154. doi:10.1002/bit.25321

Hülsen T, Batstone DJ, Keller J (2014) Phototrophic bacteria for nutrient recovery from domestic wastewater. Water Res 50:18–26

Hunter CN (2008) The purple phototrophic bacteria. Springer, Berlin

Ikumi D, Brouckaert CJ, Ekama GA (2011) Modelling of struvite precipitation in anaerobic digestion. Paper presented at the WA Watermatex2011, San Sebastian, Spain, 20–22 June 2011

Jenicek P, Keclik F, Maca J, Bindzar J (2008) Use of microaerobic conditions for the improvement of anaerobic digestion of solid wastes. Water Sci Technol 58:1491–1496. doi:10.2166/wst.2008.493

Jensen PD, Ge H, Batstone DJ (2011) Assessing the role of biochemical methane potential tests in determining anaerobic degradability rate and extent. Water Sci Technol 64:880–886

Jensen PD, Astals S, Lu Y, Devadas M, Batstone DJ (2014a) Anaerobic codigestion of sewage sludge and glycerol, focusing on process kinetics, microbial dynamics and sludge dewaterability. Water Res 67:355–366

Jensen PD, Sullivan T, Carney C, Batstone DJ (2014b) Analysis of the potential to recover energy and nutrient resources from cattle slaughterhouses in Australia by employing anaerobic digestion. Appl Energy 136:23–31. doi:10.1016/j.apenergy.2014.09.009

Jimenez J, Gonidec E, Cacho Rivero JA, Latrille E, Vedrenne F, Steyer JP (2014) Prediction of anaerobic biodegradability and bioaccessibility of municipal sludge by coupling sequential extractions with fluorescence spectroscopy: towards ADM1 variables characterization. Water Res 50:359–372

Kalyuzhnyi S, Fedorovich V (1998a) Mathematical modelling of competition between sulphate reduction and methanogenesis in anaerobic reactors. Biores Tech 65:227–242

Kalyuzhnyi SV, Fedorovich VV (1998b) Mathematical modelling of competition between sulphate reduction and methanogenesis in anaerobic reactors. Bioresour Technol 65:227–242. doi:10.1016/S0960-8524(98)00019-4

Kazadi Mbamba C, Batstone DJ, Flores-Alsina X, Tait S (2015a) A generalised chemical precipitation modelling approach in wastewater treatment applied to calcite. Water Res 68:342–353. doi:10.1016/j.watres.2014.10.011

Kazadi Mbamba C, Tait S, Flores-Alsina X, Batstone DJ (2015b) A systematic study of minerals precipitation modelling in wastewater treatment processes. Water Res (in press)

Kim MK, Choi K-M, Yin C-R, Lee K-Y, Im W-T, Lim JH, Lee S-T (2004) Odorous swine wastewater treatment by purple non-sulfur bacteria, *Rhodopseudomonas palustris*, isolated from eutrophicated ponds. Biotechnol Lett 26:819–822

Kim SY, Tojo Y, Matsuto T (2007) Compartment model of aerobic and anaerobic biodegradation in a municipal solid waste landfill. Waste Manag Res, ISWA 25:524–537

Klamt S, Schuster S, Gilles ED (2002) Calculability analysis in underdetermined metabolic networks illustrated by a model of the central metabolism in purple nonsulfur bacteria. Biotechnol Bioeng 77:734–751

Kleerebezem R, van Loosdrecht MCM (2006) Critical analysis of some concepts proposed in ADM1 54. doi:10.2166/wst.2006.525

Klein G, Klipp W, Jahn A, Steinborn B, Oelze J (1991) The relationship of biomass, polysaccharide and H2 formation in the wild-type and nifA/nifB mutants of Rhodobacter capsulatus. Arch Microbiol 155:477–482. doi:10.1007/BF00244965

Koch G, Egli K, Van Der Meer JR, Siegrist H (2000) Mathematical modeling of autotrophic denitrification in a nitrifying biofilm of a rotating biological contactor. Water Sci Technol 41(4–5):191–198

la Cour Jansen J (2011) Anaerobic digestion: technology. In: Christensen T (ed) Solid Waste Technol Manag, vol 2. Wiley, London, pp 601–617

Lei Z, Zhang Z, Huang W, Cai W (2015) Recent progress on dry anaerobic digestion of organic solid wastes: achievements and challenges. Curr Org Chem 19:400–412

Li YF, Chen PH, Yu Z (2014) Spatial and temporal variations of microbial community in a mixed plug-flow loop reactor fed with dairy manure. Microb Biotechnol 7:332–346. doi:10.1111/1751-7915.12125

Liang C-M, Hung C-H, Hsu S-C, Yeh I-C (2010) Purple nonsulfur bacteria diversity in activated sludge and its potential phosphorus-accumulating ability under different cultivation conditions. Appl Microbiol Biotechnol 86:709–719. doi:10.1007/s00253-009-2348-2

Liao BQ, Kraemer JT, Bagley DM (2006) Anaerobic membrane bioreactors: applications and research directions. Crit Rev Environ Sci Technol 36:489–530. doi:10.1080/10643380600678146

Lieberman RL, Rosenzweig AC (2004) Biological methane oxidation: regulation, biochemistry, and active site structure of particulate methane monooxygenase. Crit Rev Biochem Mol Biol 39:147–164. doi:10.1080/10409230490475507

Linke B, Rodríguez-Abalde Á, Jost C, Krieg A (2015) Performance of a novel two-phase continuously fed leach bed reactor for demand-based biogas production from maize silage. Bioresour Technol 177:34–40. doi:10.1016/j.biortech.2014.11.070

Lizarralde I et al (2015) A new general methodology for incorporating physico-chemical transformations into multi-phase wastewater treatment process models. Water Research 74:239–256. doi:10.1016/j.watres.2015.01.031

Long JH, Aziz TN, Reyes FL III, Ducoste JJ (2012) Anaerobic co-digestion of fat, oil, and grease (FOG): a review of gas production and process limitations. Process Saf Environ Prot 90:231–245. doi:10.1016/j.psep.2011.10.001

Lopes F et al (2011) Biogeochemical modelling of anaerobic vs. aerobic methane oxidation in a meromictic crater lake (Lake Pavin, France). Appl Geochem 26:1919–1932. doi:10.1016/j.apgeochem.2011.06.021

Lovley DR, Stolz JF, Nord GL, Phillips EJP (1987) Anaerobic production of magnetite by a dissimilatory iron-reducing microorganism. Nature 330:252–254

Lovley DR, Phillips EJP, Gorby YA, Landa ER (1991) Microbial reduction of uranium. Nature 350:413–416

Mata-Alvarez J, Dosta J, Macé S, Astals S (2011) Codigestion of solid wastes: a review of its uses and perspectives including modeling. Crit Rev Biotechnol 31:99–111. doi:10.3109/07388551.2010.525496

McCarty PL, Bae J, Kim J (2011) Domestic wastewater treatment as a net energy producer-can this be achieved? Environ Sci Technol 45:7100–7106. doi:10.1021/es2014264

McKinlay JB, Harwood CS (2010) Carbon dioxide fixation as a central redox cofactor recycling mechanism in bacteria.

Proc Natl Acad Sci 107:11669–11675. doi:10.1073/pnas.1006175107

Melnicki MR, Eroglu E, Melis A (2009) Changes in hydrogen production and polymer accumulation upon sulfur-deprivation in purple photosynthetic bacteria. Int J Hydrogen Energy 34:6157–6170

Munoz R, Guieysse B (2006) Algal–bacterial processes for the treatment of hazardous contaminants: a review. Water Res 40:2799–2815

Muñoz-Tamayo R, Laroche B, Walter É, Doré J, Leclerc M (2010) Mathematical modelling of carbohydrate degradation by human colonic microbiota. J Theor Biol 266:189–201. doi:10.1016/j.jtbi.2010.05.040

Nopens I, Batstone DJ, Copp JB, Jeppsson U, Volcke E, Alex J, Vanrolleghem PA (2009) An ASM/ADM model interface for dynamic plant-wide simulation. Water Res 43:1913–1923

Nopharatana A, Pullammanappallil PC, Clarke WP (2003) A dynamic mathematical model for sequential leach bed anaerobic digestion of organic fraction of municipal solid waste. Biochem Eng J 13:21–33

Overmann J, Garcia-Pichel F (1998) The phototrophic way of life: The Prokaryotes: an evolving electronic resource for the microbiological community M Dworkin. Springer, New York

Ozgun H, Dereli RK, Ersahin ME, Kinaci C, Spanjers H, van Lier JB (2013) A review of anaerobic membrane bioreactors for municipal wastewater treatment: integration options, limitations and expectations. Sep Purif Technol 118:89–104. doi:10.1016/j.seppur.2013.06.036

Pagés-Díaz J, Westman J, Taherzadeh MJ, Pereda-Reyes I, Sárvári Horváth I (2015) Semi-continuous co-digestion of solid cattle slaughterhouse wastes with other waste streams: Interactions within the mixtures and methanogenic community structure. Chem Eng J 273:28–36. doi:10.1016/j.cej.2015.03.049

Papadopoulos A, Parisopoulos G, Papadopoulos F, Karteris A (2003) Sludge accumulation pattern in an anaerobic pond under Mediterranean climatic conditions. Water Res 37:634–644. doi:10.1016/S0043-1354(02)00307-X

Pavlostathis SG, Gossett JM (1986) A kinetic model for anaerobic digestion of biological sludge. Biotech Bioeng 28:1519–1530

Peiris BRH, Rathnasiri PG, Johansen JE, Kuhn A, Bakke R (2006) ADM1 simulations of hydrogen production. 53. doi:10.2166/wst.2006.243

Penumathsa BKV, Premier GC, Kyazze G, Dinsdale R, Guwy AJ, Esteves S, Rodríguez J (2008) ADM1 can be applied to continuous bio-hydrogen production using a variable stoichiometry approach. Water Res 42:4379–4385. doi:10.1016/j.watres.2008.07.030

Pikaar I, Sharma KR, Hu S, Gernjak W, Keller J, Yuan Z (2014) Reducing sewer corrosion through integrated urban water management. Science 345:812–814

Pratt S, Liew D, Batstone DJ, Werker AG, Morgan-Sagastume F, Lant PA (2012) Inhibition by fatty acids during fermentation of pre-treated waste activated sludge. J Biotechnol 159:38–43. doi:10.1016/j.jbiotec.2012.02.001

Pullammanappallil PC, Svoronos SA, Chynoweth DP, Lyberatos G (1998) Expert system for control of anaerobic digesters. Biotechnol Bioeng 58:13–22. doi:10.1002/(SICI)1097-0290(19980405)58:1<13:AID-BIT2>3.0.CO;2-X

Puyol D, Carvajal-Arroyo J, Sierra-Alvarez R, Field J (2014) Nitrite (not free nitrous acid) is the main inhibitor of the anammox process at common pH conditions. Biotechnol Lett 36:547–551

Raghoebarsing AA et al. (2006) A microbial consortium couples anaerobic methane oxidation to denitrification. Nature 440:918–921. http://www.nature.com/nature/journal/v440/n7086/suppinfo/nature04617_S1.html

Razaviarani V, Buchanan ID (2015) Calibration of the Anaerobic Digestion Model No. 1 (ADM1) for steady-state anaerobic co-digestion of municipal wastewater sludge with restaurant grease trap waste. Chem Eng J 266:91–99. doi:10.1016/j.cej.2014.12.080

Ren T-T, Mu Y, Ni B-J, Yu H-Q (2009) Hydrodynamics of upflow anaerobic sludge blanket reactors. AIChE J 55:516–528. doi:10.1002/aic.11667

Rivera-Salvador V, López-Cruz IL, Espinosa-Solares T, Aranda-Barradas JS, Huber DH, Sharma D, Toledo JU (2014) Application of Anaerobic Digestion Model No. 1 to describe the syntrophic acetate oxidation of poultry litter in thermophilic anaerobic digestion. Bioresour Technol 167:495–502. doi:10.1016/j.biortech.2014.06.008

Robles A, Ruano MV, Ribes J, Ferrer J (2013a) Advanced control system for optimal filtration in submerged anaerobic MBRs (SAnMBRs). J Membr Sci 430:330–341. doi:10.1016/j.memsci.2012.11.078

Robles A, Ruano MV, Ribes J, Seco A, Ferrer J (2013b) A filtration model applied to submerged anaerobic MBRs (SAnMBRs). J Membr Sci 444:139–147. doi:10.1016/j.memsci.2013.05.021

Robles A, Ruano MV, Ribes J, Seco A, Ferrer J (2014) Model-based automatic tuning of a filtration control system for submerged anaerobic membrane bioreactors (AnMBR). J Membr Sci 465:14–26. doi:10.1016/j.memsci.2014.04.012

Rodriguez-Freire L, Sierra-Alvarez R, Root R, Chorover J, Field JA (2014) Biomineralization of arsenate to arsenic sulfides is greatly enhanced at mildly acidic conditions. Water Res 66:242–253

Rosen C, Vrecko D, Gernaey KV, Pons MN, Jeppsson U (2006) Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink, vol 54

Saqqar MM, Pescod MB (1995) Modelling sludge accumulation in anaerobic wastewater stabilization ponds. Water Sci Technol 31:185–190. doi:10.1016/0273-1223(95)00505-H

Saravanan V, Sreekrishnan TR (2006) Modelling anaerobic biofilm reactors-A review. J Environ Manage 81:1–18. doi:10.1016/j.jenvman.2005.10.002

Saritpongteeraka K, Boonsawang P, Sung S, Chaiprapat S (2014) Co-fermentation of oil palm lignocellulosic residue with pig manure in anaerobic leach bed reactor for fatty acid production. Energy Convers Manag 84:354–362. doi:10.1016/j.enconman.2014.04.056

Shewani A, Horgue P, Pommier S, Debenest G, Lefebvre X, Gandon E, Paul E (2015) Assessment of percolation through a solid leach bed in dry batch anaerobic digestion processes. Bioresour Technol 178:209–216. doi:10.1016/j.biortech.2014.10.017

Shilton A, Harrison J (2003) Development of guidelines for improved hydraulic design of waste stabilisation ponds. Water Sci Technol 48:173–180

Shin C, McCarty PL, Kim J, Bae J (2014) Pilot-scale temperate-climate treatment of domestic wastewater with a staged anaerobic fluidized membrane bioreactor (SAF-MBR). Bioresour Technol 159:95–103. doi:10.1016/j.biortech.2014.02.060

Siegrist H, Renggli D, Gujer W (1993) Mathematical modelling of anaerobic mesophilic sewage sludge treatment. Wat Sci Tech 27:25–36

Siegrist H, Vogt D, Garcia-Heras J, Gujer W (2002) Mathematical model for meso and thermophilic anaerobic sewage sludge digestion. Environ Sci Technol 36:1113–1123

Solon K et al (2015) Effects of ionic strength and ion pairing on (plant-wide) modelling of anaerobic digestion. Water Res 70:235–245. doi:10.1016/j.watres.2014.11.035

Spagni A, Ferraris M, Casu S (2015) Modelling wastewater treatment in a submerged anaerobic membrane bioreactor. J Environ Sci Health Part A 50:325–331. doi:10.1080/10934529.2015.981123

Stuckey DC (2012) Recent developments in anaerobic membrane reactors. Bioresour Technol 122:137–148. doi:10.1016/j.biortech.2012.05.138

Tang K, Baskaran V, Nemati M (2009) Bacteria of the sulphur cycle: an overview of microbiology, biokinetics and their role in petroleum and mining industries. Biochem Eng J 44:73–94. doi:10.1016/j.bej.2008.12.011

Thamsiriroj T, Nizami AS, Murphy JD (2012) Use of modeling to aid design of a two-phase grass digestion system. Bioresource Technology 110:379–389. doi:10.1016/j.biortech.2012.01.113

Tugtas AE, Tezel U, Pavlostathis SG (2010) A comprehensive model of simultaneous denitrification and methanogenic fermentation processes. Biotechnol Bioeng 105:98–108. doi:10.1002/bit.22443

Utgikar VP, Harmon SM, Chaudhary N, Tabak HH, Govind R, Haines JR (2002) Inhibition of sulfate-reducing bacteria by metal sulfide formation in bioremediation of acid mine drainage. Environ Toxicol 17:40–48. doi:10.1002/tox.10031

Van Hulle SWH, Vesvikar M, Poutiainen H, Nopens I (2014) Importance of scale and hydrodynamics for modeling anaerobic digester performance. Chem Eng J 255:71–77

van Niftrik L et al (2008a) Linking ultrastructure and function in four genera of anaerobic ammonium-oxidizing bacteria: cell plan, glycogen storage, and localization of cytochrome C proteins. J Bacteriol 190:708–717

van Niftrik L et al (2008b) Combined structural and chemical analysis of the anammoxosome: a membrane-bounded intracytoplasmic compartment in anammox bacteria. J Struct Biol 161:401–410. doi:10.1016/j.jsb.2007.05.005

Vavilin VA, Rytov SV, Lokshina LY (1996) A description of hydrolysis kinetics in anaerobic degradation of particulate organic matter. Biores Tech 56:229–237

Vavilin VA, Lokshina LY, Rytov SV, Kotsyurbenko OR, Nozhevnikova AN, Parshina SN (1997) Modelling methanogenesis during anaerobic conversion of complex organic matter at low temperatures. Wat Sci Tech 36:531–538

Volcke EIP, van Loosdrecht MCM, Vanrolleghem PA (2006) Continuity-based model interfacing for plant-wide simulation: a general approach. Water Res 40:2817–2828. doi:10.1016/j.watres.2006.05.011

Weijma J, Copini CFM, Buisman CJN, Schultz CE (2002) Biological recovery of metals, sulfur and water in the mining and metallurgical industry. IWA Publishing, London, pp 605–622

Wett B, Takács I, Batstone D, Wilson C, Murthy S (2014) Anaerobic model for high-solids or high-temperature digestion—additional pathway of acetate oxidation. Water Sci Technol 69:1634–1640. doi:10.2166/wst.2014.047

Wu D et al (2013) A new biological phosphorus removal process in association with sulfur cycle. Water Res 47:3057–3069. doi:10.1016/j.watres.2013.03.009

Wu D et al (2014) Simultaneous nitrogen and phosphorus removal in the sulfur cycle-associated enhanced biological phosphorus removal (EBPR) process. Water Res 49:251–264. doi:10.1016/j.watres.2013.11.029

Zaher U, Buffiere P, Steyer JP, Chen S (2009) A procedure to estimate proximate analysis of mixed organic wastes. Water Environ Res 81:407–415. doi:10.2175/106143008X370548

Zhang F, Ding J, Zhang Y, Chen M, Ding Z-W, van Loosdrecht MCM, Zeng RJ (2013) Fatty acids production from hydrogen and carbon dioxide by mixed culture in the membrane biofilm reactor. Water Res 47:6122–6129. doi:10.1016/j.watres.2013.07.033

Zhu G, Zou R, Jha AK, Huang X, Liu L, Liu C (2015) Recent developments and future perspectives of anaerobic baffled bioreactor for wastewater treatment and energy recovery. Crit Rev Environ Sci Technol 45:1243–1276. doi:10.1080/10643389.2014.924182