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J. Lauwers, L. Appels, I.P. Thompson, J. Degrève, J.F. Van Impe, R. Dewil (2013). Mathematical modelling of anaerobic digestion of biomass and waste: Power and limitations, Progress in Energy and Combustion Science, 39, 383-402.

The journal and the original published paper can be found at:

<http://www.journals.elsevier.com/progress-in-energy-and-combustion-science/>
<http://www.sciencedirect.com/science/article/pii/S0360128513000178>

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MATHEMATICAL MODELLING OF ANAEROBIC DIGESTION OF BIOMASS AND WASTE: POWER AND LIMITATIONS

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Anaerobic digestion is an excellent technique for the energetic valorisation of various types of biomass including waste forms. Because of its complex nature, the optimisation and further process development of this technology go hand in hand with the availability of mathematical models for both simulation and control purposes. Over the years, the variety of mathematical models developed has increased as have their complexity. This paper reviews the trends in anaerobic digestion modelling, with the main focus on the current state of the art. The most significant simulation and control models are highlighted, and their effectiveness critically discussed. The importance of the availability of models that are less complex, which can be used for control purposes, is assessed. The paper concludes with a discussion on the inclusion of microbial community data in mathematical models, an innovative approach which could drastically improve model performance

Keywords: Anaerobic digestion, modelling, ADM1, biogas, microbial community

1. INTRODUCTION

The mitigation of CO₂ emissions and associated global warming necessitates the exploitation of renewable forms of energy in order to reduce the dependency on fossil fuels. In this regard, energy from biomass is seen to be one of the most promising future renewable energy sources. Anaerobic digestion is a robust and efficient technology for the energetic valorization of various types of biomass (including organic wastes), and it is predicted to play a crucial role in the future of renewable energy production [1, 2]. The European Union Green Paper on the management of bio-waste further stresses the importance of anaerobic digestion for the treatment of non-combustible types of biomass. In recent years, the application of anaerobic digestion for the treatment of organic waste streams has grown spectacularly, with an annual growth rate of 25 % [1,2,3]. Although the process has been known and implemented for many decades, it is not yet fully understood. This is mainly due to the complexity of the different (microbial and physicochemical) reactions involved. Further development is needed to optimize the process, including a more fundamental understanding of the underlying mechanisms, together with the availability of mathematical models for both simulation and control purposes.

During the digestion process, a fraction of the organic matter is converted into an energy-rich biogas. In general, most organic substrates are suitable for anaerobic digestion including

wastewater sludge, the organic fraction of municipal solid waste and some types of industrial wastes (e.g. fats, oils and grease (FOG), manure, crop waste from agriculture and dedicated energy crops). Anaerobic digestion comprises a myriad of reactions, most of which are biochemical in nature. A simplified reaction scheme is depicted in Fig. 1.

The first step of the process comprises the disintegration of particulate organic matter into carbohydrates, lipids and proteins, which are further hydrolysed enzymatically (extracellular) to short chained carbohydrates, long chain fatty acids and amino acids. These hydrolytic enzymes are secreted by microorganisms, present in the bulk liquid or attached to particulates [4]. Acidogenic microorganisms subsequently convert these soluble components to alcohols and/or organic acids (e.g. acetate, propionate, butyrate, valerate), which are, in turn, converted into acetate and ultimately into methane and carbon dioxide by acetoclastic methanogens. Carbon dioxide and hydrogen (produced as intermediates) are also combined via hydrogenotrophic methanogens to generating CH₄.

The latter mechanism is responsible for about 30% of total methane production [4,5]. The resulting biogas composition depends on several factors: (i) the oxidation state of carbon in the substrate [6], (ii) the residence time, which generally is positively correlated with the methane content, (iii) the reactor set-up (a continuous digestion favours lower CO₂ content because of discharge of dissolved CO₂ in the liquid) and (iv) the temperature, which changes the overall kinetics and solubility of gases.

Dissolved hydrogen is a key variable in the digestion process: high concentrations inhibit the acidogenesis/acetogenesis phases while it is a necessary component in hydrogenotrophic methanogenesis [7]. The complete reaction network is much more complicated and includes, for instance, the reduction of sulphur and nitrates, and the oxidation of methanol and formate, the degradation of siloxanes and the formation of lactic acid. Additionally, acid–base equilibria and vapour–liquid mass transfer should also be taken into account, as well as microbial growth and decay [8].

Anaerobic digestion is still the subject of intensive research, specifically focused on novel digester design, substrate pre-treatment to improve the biodegradability of the biomass (hence enhancing the biogas production) and upgrading of the biogas [1,9]. Also, only recently developed advanced culture independent molecular techniques for identification of the microbial communities have paved the way for obtaining more fundamental insights in the process [10].

In parallel with novel process developments and experimental research, considerable effort has been put into the mathematical modelling of anaerobic digestion. There is general agreement in the literature that the development of mathematical models results in a better understanding of the process dynamics, reveals optimisation opportunities and is an overall prerequisite for improvement of digester performance.

In general, there are two types of model classifications: dynamic or non-dynamic and white-box, grey-box or black-box. The first refers to the time-frame of the model predictions. Dynamic models are capable of making predictions continuous in time or at least at regular discrete intervals, while the non-dynamic models only predict time-independent variables.

The distinction between white-box, grey-box and black-box models is based on the amount of a priori information included. White box models are deductive, and use a priori information to describe the biochemical reactions occurring during digestion. In contrast,

black-box models, or data-driven models inductively link the input directly to the output without including any prior knowledge of the physical and chemical reactions occurring. Grey-box or mechanistically inspired models are those in which the parameters have a physical interpretation but are adjustable, for instance by a parameter estimation procedure. This is often the result of an approximation or simplification of the described process. Because anaerobic digestion processes are of significant complexity most dynamic models are of this type.

Dynamic models consist of several ordinary differential equations (ODE), based on mass-balance considerations. The ODE are mostly of the form of equation (1) in which ξ is the vector of state variables such as concentration of components and active anaerobic biomass, $\mathbf{D}$ (d^{-1}) is the dilution rate, i.e. the ratio between volumetric inflow ($d^{-1}m^3$) and digester volume of the digester liquid (m^3), $\mathbf{K}$ is the stoichiometric or rate-equation matrix, $\mathbf{r}(\xi)$ is the reaction rate matrix, and $\mathbf{F}(\xi)$ the mass-transfer dynamics which mostly involve gas-liquid interactions

$$\frac{d\xi}{dt} = (\xi_{in} - \xi)\mathbf{D} + \mathbf{K}\mathbf{r}(\xi) - \mathbf{F}(\xi) \quad (1)$$

In addition to the ODEs, also algebraic equations (AE) are required in most model structures. These originate from mass or charge balances or from instantaneous reactions (e.g. neutralization reactions, flow of insoluble gaseous components).

Non-dynamic white-box models link substrate to products on stoichiometric grounds. Generally, they can be calculated by Equation (2) for the elements C, H, O and N [11].

However, the occurrence of non-biodegradable biomass and the concurrent growth of biomass complicate this stoichiometric approach [12]. Consequently, this approach is not commonly employed and as such not further discussed in this review.

A specific class is experience-based models that are dependent on large amounts of a priori information, but have a totally different structure compared to typical white-box models. Because of the need of an extensive data-base, that expresses this experience, they can be classified as data-driven.

This paper critically reviews the development of anaerobic digestion modelling, with the main focus on the current state of the art. In Section 2 some fundamentals concerning modelling are presented. In Section 3, mechanistically inspired models are discussed, whereas the use of models in control applications is reviewed in Section 4. Section 5 includes data-driven models. In the final section, the future needs in anaerobic digestion modelling are highlighted.

2. MODELLING OF ANAEROBIC DIGESTION: FRAMEWORK

The general framework for the use of a mathematical model is a 6-step procedure depicted in Fig. 2 [13,14].

In the first model selection step, a trade-off should be made between accuracy and model complexity (the latter is determined by the number of state variables and parameters included). It is also here where a choice has to be made between data-driven or mechanistically inspired models. This initial choice of type and specifics of a model is partially driven by the amount of a priori knowledge available on the system.

The next step is the parameter selection for calibration. Principally, this selection should be based on an evaluation of the identifiability of the specific parameters, i.e. the ability to determine parameter values univocally. Identifiability encompasses structural or theoretical components, assuming the state variables are completely impartially known in time and the practical identifiability, taking into account measuring noise and sampling frequency. Several methods for analysing identifiability are available [14]. If the identifiability of the parameters cannot be examined, the next best option is to examine the parameter sensitivity. Although the global sensitivity can be calculated [15], analysis of the local sensitivity is more common [16,17]. In some cases, parameter values can be taken from the literature if the conditions of the experiment are sufficiently similar to the previously reported ones, and/or when the parameter demonstrates little variability [4].

The third step in the modelling procedure is the data collection, i.e. experimental measurements. A specific problem for anaerobic digestion is the challenge of spatial and temporal quantification of the specific microbial populations that are active in the system at any one time. Some advanced molecular techniques employed to identify the presence and activity of microbial community members have been developed recently, but are not yet frequently applied in anaerobic digestion research. Alternative options for dealing with the issues of uncertainty with regards the biomass include: (i) assuming constant biomass composition [18], (ii) assigning a fixed fraction of volatile suspended solids (VSS) to each microbial group [19], (iii) estimating the initial biomass concentration from a preliminary simulation of the digester or by including them in the parameter estimation [13] and (iv), using state-estimators, based on the measurement of other variables [20, 21].

Various cost functions or objective functions have been used for the parameter estimation such as least squares, least-modulus, or maximum likelihood [13]. Also, a large number of minimisation algorithms have been applied: Gauss–Newton, the steepest-descent method, Levenberg–Marquardt (combination of Gauss–Newton and steepest descent), and genetic algorithms to name a few [14, 15].

In the subsequent accuracy estimation, the uncertainty is determined. This is expressed by the measurements' covariance matrix and the previously determined sensitivity. Confidence intervals for the estimated parameters can also be developed [14]. If the estimated uncertainty is too large, additional experiments should be carried out. The experiment, however, can itself be optimised in a design of experiments, to deliver the most information on the parameter estimates [22].

In practice, a single test with the intended substrate (for instance sludge) will not yield enough information to determine all the parameters with sufficient reliability. The cause for this problem is that the overall rate of the digestion process is often determined by the slowest process. Typically, the disintegration-hydrolysis is rate-limiting for substrates that contain

large quantities of particulates, while the methanogenesis step is considered to be the slowest for dissolved substrate. In those cases, a proper design of the experiment to estimate the parameter relating the non-limiting kinetics is impossible. As a result, two options are available: perform an additional test in which intermediate degradation components are added, or rely on previously reported parameters. A good example of the first option is given by the activity measurements provided by Regeuero et al. [23], whilst most of the articles mentioned in this review use previously reported parameters.

Finally, the resulting model should be subjected to a validation procedure, both of the calibration and independently obtained data.

Validation is often reported in terms of the coefficient of determination, R^2 [13, 24]. A visual inspection, in which the trend of the predictions is compared with the measurements, can also be helpful. If the results are not satisfactory, the quality of the data has to be improved by designing new experiments or employing alternative model structures. What is deemed to be 'a good model' is of course dependent on its intended purpose.

With regards the accuracy of the model structure, Ljung [25] gives some practical tips and tools to assess its validity. Considerable information can be obtained by analysing the residuals. If the model is correct, i.e. a reliable representation of the reality, the obtained residuals of validation of the model should be independent random variables. This can be tested by a Whiteness test in which a derived form of the residuals should obey a χ^2 -distribution. Alternatively, the residuals should not show any correlation between themselves or with past inputs. If the latter were true, this means that in the residual, the input can be 'seen', or that a part of the measured output is not detected by the model. A criterion for evaluation is to check whether the correlation between the inputs and the residuals is significantly different from the correlation within the residuals as well as the inputs.

3. MECHANISTICALLY INSPIRED MODELS

Dynamic white-box models aim to accurately describe the dynamic processes occurring during digestion. This requires a measurement of the major components in the digestion system and, as a result, the use of lumped variables (i.e. variables that represent a combination of different components) is not sufficient. Because of the complexity of anaerobic digestion, the number of variables and associated number of equations included in a model can be very high (a large variety of carbohydrates, proteins and amino acids, fats, long chain fatty acids (LCFA), volatile fatty acids (VFA), alcohols, esters, and aldehydes are typically present) and in most cases it is impractical to include all the parameters that may be influencing the digestion. This observation necessitates the requirement to select those components and reaction pathways that are deemed to be important. For these reasons the grey-box models are more suitable for the purpose of modelling the anaerobic digestion process.

3.1 Overview of anaerobic digestion models

The first anaerobic digestion models date back to the mid-sixties with the model proposed by Andrews and Pearson [26]. The substrate of the digestion was assumed to consist of dissolved organic substances, which were converted to methane by microbial acidogenesis and acetoclastic methanogenesis. Because the latter is rate-limiting for solutes, several models

have been developed, that estimate biogas production using only the methanogenesis step [27, 28]. Denac et al. [29] extended these models by including acetogenesis for the conversion of propionate into acetate. The kinetics of these steps is traditionally expressed by Monod type kinetics, which consider a single growth-limiting substrate (equation (3)):

$$\mu = \mu_{\max} \frac{[S]}{[S] + K_S} \quad (3)$$

with μ (d^{-1}) the specific growth rate, $\mu_{\max}$ (d^{-1}) the maximum specific growth rate, $[S]$ ($g\ L^{-1}$) the substrate concentration, and K_S ($g\ L^{-1}$) the substrate saturation constant (i.e. substrate concentration at half $\mu_{\max}$).

It was found, however, that the acetoclastic methanogenesis step exhibited inhibition at high concentration of acetate [27]. Accordingly, a kinetic equation was proposed, based on Haldane kinetics (equation (4)), as given in equation (5). The latter is sometimes referred to as “Andrews kinetics” [30],

$$\mu = \frac{\mu_{\max}}{1 + \frac{K_S}{[S]} + \frac{[S]}{K_I}} \quad (4)$$

$$\mu = \frac{\mu_{\max}}{1 + \frac{K_S}{[S]} + \frac{[VFA]}{K_I}} \quad (5)$$

where $[VFA]$ ($g\ L^{-1}$) is the unionized VFA concentration, and K_I ($g\ L^{-1}$) the inhibition constant.

As knowledge of anaerobic digestion has increased, it has been clear that a range of factors can influence digestion efficiency, such as digester overloading or the occurrence of toxic components such as sulphide, ammonia or heavy metals [31]. Consequently, these inhibition effects are included in more recent models.

Because of the implicit pH dependence of these models, the H^+ concentration is calculated from the charge balance of the components included in the model. In its most extensive form, this would be represented by the equation (6).

$$[H^+] = [HCO_3^-] + \sum [VFA^-] + [LCFA^-] + [OH^-] + [An^-] - [Cat^+] - [NH_4^+] \quad (6)$$

where $[An^-]$ and $[Cat^+]$ are the anion and cation concentrations.

To obtain realistic pH calculations and biogas production rates, it also became necessary to account for the solubility of CO_2 in water and its mass-transfer to the gas phase, as in Equation (7)

$$r_{CO_2} = k_L a \left(\frac{P_{CO_2}}{H_{CO_2}} - [CO_2] \right) \quad (7)$$

where r_{CO_2} ($\text{g L}^{-1} \text{d}^{-1}$) represents the liquid–gas mass transfer, $k_l a$ (d^{-1}) the mass-transfer constant, P_{CO_2} (Pa) the partial pressure of CO_2 in the gas-phase, H_{CO_2} the Henry constant (Pa mol^{-1}) and $[\text{CO}_2]$ (g L^{-1}) the concentration of unionized CO_2 in the liquid phase. This equation can also be used for other gases, for example H_2 and CH_4 , but is less common due to their low solubility.

Some models specifically address the degradation of glucose [32-34]. Although not very relevant for practical applications, they are of interest from a research perspective. Mosey [32] investigated metabolism regulation by hydrogen, by expressing the concentrations of NADH/NAD^+ , whilst Kalyuzhnyi [34] expressed the ethanol generation and degradation pathway.

The digestion of dissolved organics, however, is not a very realistic situation because most non-synthetic substrates are (at least partially) particulate in nature. Therefore, the acidogenic and methanogenic step are preceded by a hydrolysis step in which these are solubilised. This step is rate limiting in most practical digestion situations (especially when a significant portion of particulates is present) [35-37].

Several kinetic equations for hydrolysis are reported in the literature [37 - 40], such as surface-based and Contois kinetics. Most models, however, consider hydrolysis to be a first-order reaction. It should be pointed out that such first-order hydrolysis kinetics are mostly only apparent first-order and the kinetic constants can vary widely depending on various factors such as the prevailing type of microorganisms or changes in particle size distribution [4, 38, 41].

Sanders et al. [38] proposed a surface-based kinetic expression, describing the coverage of particles with bacteria that secrete hydrolytic exo-enzymes. With this the hydrolysis constant per unit area remains constant in order to account for the variable concentrations of enzyme. This is represented in the equation (8).

$$\mu = k_{\text{SBK}} A \quad (8)$$

where k_{SBK} ($\text{g m}^{-2} \text{d}^{-1}$) is the surface based hydrolysis constant and A (m^2) is the surface area available for hydrolysis.

A model that makes use of surface-based kinetics has been developed by Hobson [42]. This type of kinetics can also be made particle shape dependent, as explained by Vavilin et al. [43].

According to Vavilin et al. [37], hydrolysis is a two phase process. In the first phase the particulates are colonised by bacteria, which subsequently excrete the hydrolytic enzymes. When a surface is covered with bacteria, it degrades at a constant depth, per unit of time. This type of behaviour can be modelled effectively employing Contois-kinetics, i.e. equation (9).

$$\mu = \mu_{\text{max}} [X] \frac{[S]}{K_s [X] + [S]} \quad (9)$$

For low $[S]/[X]$, this equals a first-order equation for the substrate and for high $[S]/[X]$, this equals a first-order equation for the biomass.

Based on the implementation of Mosey [32] and Hobson [42], the hydrogenotrophic methanogenesis component was included in the models, which, in normal situations, accounts for about 30% of the CH_4 production. The inclusion of H_2 as a variable introduces a subtle system of balances in the model. On the one hand, acetogenesis, which reduces H^+ to H_2 is thermodynamically favoured by low H_2 concentrations, whilst in contrast hydrogenotrophic methanogenesis favours elevated H_2 atmosphere. This phenomenon, which is essentially a thermodynamic issue, is mostly accounted for by inclusion of a non-competitive H_2 -inhibition term in the kinetics [34, 44, 45].

Further model development addressed the digestion of more specific types of substrates: (i) wastewater, (ii) sludge, (iii) manure and (iv) solid wastes.

The modelling of anaerobic wastewater (i) treatment closely follows the evolution of the models that describe the digestion of dissolved organics and particulates. However, to account for the large variation in water pollutants, it became necessary to distinguish between the substrate components (carbohydrates, proteins and lipids) fed to the digester. In previous models these were lumped together and simply expressed as the COD. Each particulate type is then described by their specific kinetics and stoichiometry. [44,46,47]. Although the feed is considered liquid, suspended particulates are included, with accompanying hydrolysis kinetics. For readily degradable substrates (monosaccharide rich water), lactic acid may be generated and is therefore included in some models [44,45]. Models that specifically address the digestion of wastewaters are reviewed by Batstone et al. [48].

Sludge is a complex and heterogeneous matrix of components most of which are in the form of particulates. Typically, sludge can be considered as a particulate waste and as such, a hydrolysis step is required in the degradation process. It should, however, be noted that this is not entirely correct. First, the cells have to die and their content to leak out, i.e. lysis, before hydrolysis of particulates can occur. This is correctly identified by Pavlostathis and Gossett [41] who included a cell death/lysis step prior to hydrolysis.

During digestion of sludge (ii), hydrolysis/cell death and lysis are the rate-limiting steps for methane production. This was accounted for in the model proposed by Eastman and Ferguson [35]. Later variants of the model included additional steps, i.e. acidogenesis, acetogenesis and (acetoclastic and hydrogenotrophic) methanogenesis, and distinguished between the different types of particulates (carbohydrates, lipids, proteins and inert substrates). If the organic sludge loading in the digester is high, the ammonia and ammonium concentration may also increase significantly. Therefore, ammonia inhibition of acetogenesis and acetoclastic methanogenesis are included as key parameters in the model of Siegrist et al. [49]. A unique approach is that of Shimizu et al. [50] who included nucleic acids as a variable. Modelling of the sludge digestion is reviewed by Tomei et al. [51].

Digestion of animal waste and manure (iii) is characterised by high concentration of inorganic nitrogen, i.e. NH_3 , NH_4^+ , NO_2^- , NO_3^- , which is converted during the digestion process to ammonia and high concentrations of organic acids (VFA and LCFA), both of which have significant inhibitory effects on digestion [52]. Angelidaki et al. [53, 54] investigated the effects of both inhibitors and emphasised the buffering capacity of manure in their pH calculation, which is essential for modelling this substrate.

Solid waste digestion (iv) has to be treated as a special case compared to the other substrate digestion models. This is due to the lack of (sufficient) liquid medium in such systems, which

causes the hydrolysis/acidogenesis and methanogenesis steps to occur in different spatial zones [55]. Kalyuzhnyi et al. [56] considered this digestion type as a mix between seed particles with high activity and waste particles with low methanogenic activity. Biomass growth is modelled using equation-based kinetics, which are essentially slightly altered Michaelis–Menten kinetic expressions, to ensure that no thermodynamically impossible reactions occur. A full deterministic modelling approach, however, requires a distributed parameter model and evaluation of partial differential equations [55, 57]. Based on the previous experiences of specific substrate types, generally applicable models have been developed [4, 58]. These are amalgamations of the most frequently occurring effects (such as NH_3 inhibition, pH modulation, long-chain fatty acids (LCFA) inhibition, H_2 inhibition/regulation) and can act as starting points for almost all modelling problems. These models are substrate specific in terms of application (lipids, carbohydrates, proteins, specific organic acids such as propionic acid and valeric acid).

The most frequently cited models reported in the literature are presented in Table 1.

3.2 Anaerobic Digestion Model No.1 (ADM1)

The wide variety of developed models led to the realisation that action was required to converge and consolidate the enormous array options available. With this objective, the ‘IWA Task Group on Mathematical Modelling of Anaerobic Digestion Processes’ developed the Anaerobic Digestion Model No. 1 (ADM1), as a unified base for modelling of anaerobic digestion [4]. The nomenclature, units and model structure utilised are consistent with the previously published literature and the Activated Sludge Models ASM1, ASM2, and ASM3 [81]. ADM1 has (in the mean time) become available in Matlab and Simulink, but also in specific water related simulation software, such as WEST, BioWin and Aquasim.

ADM1 describes the reactions occurring in anaerobic digestion, by assuming a perfect mixture. The components are expressed in terms of their Chemical Oxygen Demand (COD) (kg COD m^{-3}). The model includes both biochemical and physicochemical processes. The biochemical reaction scheme, as applied in the model, is depicted in Fig. 3 and includes: (i) an extracellular disintegration step that converts composite particulate matter into carbohydrates, lipids, proteins and inert compounds, (ii) an extracellular enzymatic hydrolysis step that converts the degradation products into their chemical building blocks, i.e. monosaccharides, long chain fatty acids (LCFA) and amino acids (AA), (iii) acidogenesis or fermentation of the building blocks into hydrogen, acetate and volatile fatty acids (VFA), i.e. propionate, butyrate and valerate, (iv) acetogenesis of VFA to acetate and (v) acetoclastic and hydrogenotrophic methanogenesis. All biochemical extracellular steps are assumed to be of first-order, while the intracellular biochemical reactions use Monod-type kinetics for substrate uptake, accompanied by biomass growth. Death of the biomass is represented by first-order kinetics, with the dead biomass considered as composite particulate matter. Inhibition of the biological activity by pH (all groups), hydrogen (acetogenesis) and free ammonia (acetoclastic methanogenesis) are also included. Inorganic carbon and nitrogen, i.e. CO_2 , HCO_3^- , NH_3 , NH_4^+ , act as source-sink terms and effectively close the mass balance for C and N.

Implementation of ADM1 includes 2 ODEs for cations and anions, 3 ODEs for CH_4 , H_2 and CO_2 in the vapour phase, 12 ODEs for CH_4 , H_2 , carbohydrates, lipids, amino acids, valeric acid, butyric acid, propionic acid, acetic acid, inorganic carbon and nitrogen and soluble inert

components, 4 ODEs are dedicated to the particulate matter and its lipid, protein, carbohydrate and inert contents, 7 ODEs for the microbial groups: sugar degraders, amino acid degraders, fatty acid degraders, butyrate/valerate degraders, propionate degraders and acetoclastic and hydrogenotrophic methanogens. Acid–base equilibrium for inorganic carbon and nitrogen, acetate, propionate, valerate, butyrate and hydrogen is calculated in two ways: (i) formulation of either the base or acid concentration in ODE's or (ii) calculation of the equilibrium in algebraic equations. Additionally, to reduce the rigidity of the system, the hydrogen content of the biogas can also be expressed in an algebraic equation [82].

In the literature, 3 variants of ADM1 are available: (i) the standard description STR-13, given by the IWA Task Group for Mathematical Modelling of Anaerobic Digestion Processes [4], (ii) the COST version [82, 83] which is further used in the application mentioned in Section 3.3 and (iii) the CEIT version for plant-wide modelling (PWM), i.e. ADM1-PWM [84 - 86], which is further explained in Section 3.3.

The array of versions or descriptions differ a little, and the differences mostly account for deficiencies in mass balances of the model by modifying the elemental composition of particulate matter and inert components: STR-13, using the suggested stoichiometric and composition variables, has a complete mass-balance for Carbon Oxygen Demand, i.e. all the COD can be accounted for. However, as pointed out in [82], using the default parameters leads to an imbalance in inorganic C and N which could give unrealistic predictions of the biogas composition and ammonia content. Notably, the nitrogen content of biomass and particulates differ, although this difference is not described in the equations. In the COST version, the stoichiometric coefficients, biomass degradation equations and composition parameters are adjusted accordingly to balance COD, C and N. Naturally, if one wants to use ADM1 for its own specific conditions, rather than simulating it independently, the parameters should be estimated. In this case, care has to be taken that the parameters are not chosen independently because the balances for the considered elements should be in order and ADM1-PWM generalises this in 6 conservation equations for the elements C, H, N, O, P and charge for each process. To accommodate this, additional source-sink state variables are introduced: water, dihydrogen and phosphate. Hydrogen cations are used as a dynamic charge source-sink state variable, expressed as an ODE. Because of the expression of all acid–base equilibrium as ODE's including hydrogen cation/water, algebraic calculation of the charge balance, and measurement of the cations and anions (or the difference between the two) are not necessary.

To address the differences between particulates and biomass, the ADM1-PWM considers the process of degradation of biomass to be distinct from the process of degradation of substrate particulates, expressed with its own stoichiometric coefficients. Furthermore, water evaporation is included in the model.

For newcomers to ADM1, both COST as ADM1-PWM can be appealing as they are well documented in the description of the full equations or in a complete Petersen matrix. Based on this, self implementation of the model is not difficult, and can be employed in Simulink/Matlab and in WEST.

3.2.1 Applications of ADM1

Many applications of ADM1 have been reported in the literature for a wide variety of substrates, e.g. grass silage [87], municipal waste mixed with activated sludge [88], olive mill wastewater mixed with solid waste [89], blackwater [90], cyanide-containing substrate [91], microalgae [92], mixtures of manure and vegetable waste [93], and thermally pre-treated sludge [94]. ADM1 is also applicable for simulating fermentation to hydrogen, although it is necessary to make the stoichiometry of the glucose degradation dependent on the organic acid concentration [95, 96]. It can also be used as a tool for optimisation, as was reported by Zaher et al. [97]: they determined the optimal ratio between different solid waste streams and their hydraulic retention times to maximise the biogas production rate.

3.2.2 Modifications of ADM1

The original ADM1 structure has the advantage that it serves as a platform for further modification which leads to refinement of the model. Most modifications are dedicated to specific situations or substrates, e.g. the occurrence of high concentrations of cyanide [91] or sodium [98], although some are generally applicable, such as a thermodynamic dependence of the stoichiometry [99, 100]. Considerable effort has been put into the modelling of solid or particular waste digestion. Modifications are then often focused on hydrolysis kinetics [92, 94]. An overview of adaptations of ADM1 and their field of application are presented in Table 2.

Some effort has been made to model the mass-transfer in a mixture through a distributed parameter model. Batstone et al. [101] for instance, modelled a biofilm digestion system and Mu et al. [102] an upflow anaerobic sludge bed (UASB), using a 1D discretisation. Anaerobic digestion in biofilms on granules, using a 2D and 3D discretisation, has been reported by Picioreanu et al. [103] and Batstone et al. [104]

3.3 Modelling of anaerobic digestion as a unit in a plant

Although most researchers study anaerobic digestion as an isolated process, it is often part of a plant-wide network. This is especially true for wastewater treatment plants (WWTP) in which thickened activated sludge serves as the feed to the digester and the resulting digestate supernatant is recycled to the biological wastewater treatment. Two major applications or methodologies are used in this concept, (i) the Benchmark simulation model no. 2 and (ii) the plant-wide-modelling methodology.

The Benchmark simulation model no. 2 (BSM2) is depicted in Fig. 4 [82, 83, 118, 119]. In this plant-wide modelling, anaerobic digestion is combined with a primary clarification, activated sludge system, secondary clarifier, thickener, dewatering element and a storage tank. The purpose of BSM2 is to provide a representation of a real activated sludge plant of 100,000 population equivalents, on which control strategies can be evaluated. It consists of a primary clarifier, five-reactor activated sludge system modelled with ASM1 [81], secondary clarifier, gravitational thickener, anaerobic digester, dewatering module and storage tank (Fig. 4).

Because the substrate definition differs between ASM1 and ADM1, a crucial element is the interfacing between the two models. This is a very complex matter, and a high level of specialisation is required. Only the main aspects are discussed. For a more detailed treatment, the reader is referred to the more specialised literature. The interfacing between ASM1 and ADM1 is done in six steps:

- (1) negative COD (dissolved oxygen (S_{DO}) and nitrate (S_{NO})) is subtracted from readily degradable matter (S_S), slowly degradable matter (X_S), heterotrophic biomass (X_{BH}) and autotrophic biomass (X_{BA}),
- (2) S_S and organic nitrogen (S_{ND}) are allocated to amino acids (S_{AA}), remaining S_S is allocated to monosaccharides (S_{SU}),
- (3) X_S and particulate organic nitrogen (X_{ND}) is allocated to proteins (X_{PRO}) with the remaining X_S converted to 70% lipids (X_{LI}) and carbohydrates (X_{CH}),
- (4) the activated sludge biomass consisting of biodegradable and non-degradable components
- (5) the degradable part is converted to proteins, using nitrogen in the sludge or remaining X_D , with the remainder converted to lipids and carbohydrates. The inert ASM1 components (biomass decay products X_p , inert soluble S_i , particulate X_i and the non-degradable biomass) are converted to the ADM1 inerts (S_i and X_i) taking nitrogen into account for the differences in nitrogen content, the remaining nitrogen is allocated to the inorganic nitrogen.
- (6) from S_{NO} , ammonia (SH) and the alkalinity (S_{alk}), the inorganic carbon content (SIC) and the cations ($Scat$) and anions (San) are calculated using the charge balance.

The ADM1/ASM1 interface is mainly the inverse of the ASM1/ADM1 interface. Peculiarities are the allocation of the 7 ADM1 biomass groups (X_{AA} , X_{H2} , X_{FA} , X_{C4} , X_{AC} , X_{SU} , X_{PRO}) to X_S and X_{ND} and the inclusion of the VFA (acetate S_{AC} , propionate S_{PRO} , butyrate S_{BU} and valerate S_{VAL}) in the charge balance leading to the calculation of S_{alk} . The interfacing is depicted in Fig. 5.

Up to now, the activated sludge model ASM1 has been implemented in BSM2. More developed models are available, such as ASM2, ASM2d and ASM3 [81] which include phosphorus removal. Phosphorus is of importance for anaerobic digestion as it can be a limiting substrate in anaerobic biomass growth. An interesting addition to BSM2 would be the inclusion of sulphur compounds (SO_3^{2-} , SO_4^{2-} , organic sulphur), which are converted in the digestion to H_2S .

Contrary to the use of standard models for each subunit, the whole plant (and subsequently, each unit process) can be described by considering all possible variables and apply mass-and/or energy-balances. This can be a default large number to give a *supermodel* although it can be user-selected, to address the specific purpose and plant lay-out. An example of the latter is given by the plant-wide modelling methodology, described by Grau et al. [85] that acts as a database out of which process units can be selected to construct a customised plant. First the biological processes to be included in the plant are selected, e.g. anaerobic digestion, acid fermentation, etc. Based on this choice, the necessary microorganism populations as well as physico-chemical interrelations, such as acid-base reactions are automatically selected. This will determine the set of model components combined in the *plant components vector*, used in the separate unit-process models and the transformations occurring in the selected process, e.g. anaerobic uptake of sugar or aerobic uptake of acetate. In a next step, the mass and energy balance is set-up in each process unit, using the plant components vector. Because the elemental composition for C, N, O, H, P and the charge are listed, a mass-balance over the whole of the plant can be calculated.

Although for the single anaerobic digester the result will be equivalent to a normal ADM1, it is an interesting framework for further development and extensions, both in adding new process units or additional transformations. Interestingly, this is quite clear from the example given by de Gracia et al. [86] who use this methodology for modelling of mesophilic, thermophilic and autothermal thermophilic anaerobic digestion.

4. REDUCED COMPLEXITY MODELS FOR CONTROL

As anaerobic digestion technologies mature and with large-scale plants already built, the development of efficient control strategies has become essential. Because of the complexity of the process and the delicate balance between the different degradation steps and substrate inhibition, the practical realization of those strategies is not as easily achieved as in the normal process industry [36, 121, 122].

Two goals can be distinguished for the control actions: to guarantee a stable operation and to maximise the yield for products such as hydrogen, ethanol, organic acids, or a biogas with sufficient caloric value, with the former being the most prevalent.

Direct control actions, such as a proportional–integral–derivative control (PID), can be suitable for stabilizing the digestion. For instance, alkalinity/pH levels can be stabilized by the addition of bicarbonate [123] or by altering the feed inflow [124]. This simple feed-back, however, is not very suitable for varying feed conditions such as the transition from protein to carbohydrate rich feed, which leads to a decrease in pH and NH_3 content. Additionally, a PID-type of feed-back lacks the long-term time-frame, required for product optimization and it is limited to single input and output cases.

In contrast to stabilizing actions, extremum-seeking controllers, in order to maximise the yield, have been developed. The most important examples of these types are the advanced control by disturbance monitoring by Steyer et al. [125] and state-variable feedback gain control by Liu et al. [126] and Alferes and Irizar [127].

Model-based controllers are, in that aspect, superior because the included model provides it with a robustness that helps to deal with a variety of conditions.

In theory, all models discussed in the previous section are applicable in a control action. In practice, however, implementation is hampered by the lack of on-line measuring devices. Another problem in executing control strategies is the accurate monitoring and controllability of the process. On-line monitoring is still mostly confined to pH, COD, alkalinity, total VFA and biogas composition, although some components, such as acetate, phosphorus and nitrogen can also be analysed by spectrometry [128]. Due to the rather slow kinetics of the process and increasing computational power, the mathematical complexity is, even for complex models, not a significant issue [97].

As a result, model based controllers are mostly relatively simple, with the most effective ones developed by Bastin and Dochain [66] and Bernard et al. [19].

The model of Bastin and Dochain [66] is not specific for anaerobic digestion, as it just describes the conversion of substrate to biomass with the reaction:

with X and S being the biomass and substrate, respectively. The reaction rate is proportional to biogas production [129]. The reaction rate equation can differ according to the application, although Monod-kinetics are customary [129, 130]. Parameter estimation quality for this model using Monod, Haldane and Contois kinetics are discussed by Simeonov [67].

Because of its simplicity, applications are limited to controlling the feed to prevent wash-out. This control goal is elaborated in several approaches, listed in Table 3.

The model of Bernard et al. [19] is slightly more complex. It consists of a two step mass balance model with the following reactions occurring:

Acidogenesis (with reaction rate $r_1 = \mu_1[X_1]$):

Methanogenesis (with reaction rate $r_2 = \mu_2 X_2$):

$[X_1]$ (g L^{-1}) and $[X_2]$ (g L^{-1}) are the concentrations of the acidogenic and methanogenic biomass, $[S_1]$ (g L^{-1}) and $[S_2]$ (mmol L^{-1}) the amount of organic substrate and volatile fatty acids. The acidogenic and methanogenic reaction rates are described by Monod and Haldane kinetics, respectively. The flow rates of CO_2 and CH_4 , as well as the pH-value, are calculated by algebraic equations involving the VFA and bicarbonate concentrations and the alkalinity of the liquid. Because of the absence of hydrolysis, it is valid for situations with negligible amounts of substrate particulates.

It has been demonstrated that the model developed by Bernard et al. [19] follows a scheme of developing parsimonious biochemical models, based on the eigenvalue decomposition of reaction data [133]. This eigenvalue decomposition can also be applied to cases of anaerobic hydrogen production [134]. Several control applications of the model of Bernard et al. [19] are presented in Table 4.

A final control model of interest is the 4th order model given by Simeonov et al. [139] which, like the model of Bernard et al. consists of two biomass groups. Unlike the model of Bernard et al., both are described by Monod-kinetics. Simeonov et al. [139] describe the pattern of feeding necessary to optimize methane production.

Some of the mentioned applications use software sensors, i.e. *softsensors* or *i*. Softsensors use the model structure to predict or calculate certain unknown or unreliable aspects, such as unknown state variables or reaction kinetics. A detailed discussion of softsensors lies beyond the scope of the present paper and the reader is referred to an excellent review by Dochain [140] for more information on this topic.

5. DATA DRIVEN MODELS

The models previously discussed are all based on equations expressing a mass-balance. A totally different branch of models exist, however, that do not express this conservation of mass, but model the behaviour of the system without any pre-knowledge of the occurring processes. This behaviour can also be quantified in data or expressions that reflect experience. The former are black-box models, while the latter are mostly fuzzy-logic based models.

5.1 Black-box models

The finality of data based or black box models differs largely from the mechanistic models previously discussed. Although the latter are in fact also partially based on data (for the estimation of the parameters), they are built around a generic structure for which the parameters have been trained in such a way that the resulting input–output mapping of the model is deemed optimal. For black box models, in contrast, their generic structure does not take into account (in most cases) the chemical, physical and microbial processes occurring. This kind of approach is of interest when the goal is to obtain predictions of only a few specific output variables.

Examples of some tools for the development of black-box models are (i) Principle Component Regression (PCR) [141] (ii) Partial Least Squares (PLS) [142], (iii) Artificial Neural Networks (ANN) [143], (iv) Neuro-fuzzy Systems [144] and (v) Support Vector Machines (SVM) [145]. In the field of anaerobic digestion, ANN and PLS are used.

Artificial Neural Networks, based on biological neurological systems, are time-discrete models constructed from a large number of inter-connected processing elements. These elements, neurons, are ordered in different layers of which the first and the last are assigned to the input and the output variables. The training involves determining the number of layers, interneuron connections and the connections' weights. The number of neurons and input and/or input-combinations are also model parameters. For more information on ANN, the reader is referred to Zupan and Gasteiger [146].

ANN can be used for strict predictive application, e.g. predicting biogas production [147], trace elements NH_3 and H_2S [148] or for control purposes. For example, Holubar et al. [149] controlled the loading rate of a Continuous Stirred Tank Reactor (CSTR) type digester to achieve maximal methane production and influent degradation, under the constraints of maximum VFA and minimum pH. Therefore, a hierarchical controller was developed in which two ANNs predicted VFA and pH concentration and a third one predicted biogas volume and composition. Training was done in steady-state conditions with an organic loading rate of about $2.5 \text{ kg COD/m}^3\cdot\text{day}$ using feed-forward back propagation. Regular shock load pulses of substrate were fed to the digester. Interestingly, the model was able to cope with unstable start-up phases [150]. It should be pointed out, however, that training of such a model requires a large data set, e.g. 500 days for Holubar et al. [149, 150].

Partial Least Squares (PLS), like PCR, projects the data on orthogonal components. Pairs of components in the input and output are selected in order to maximise the covariance between the two. Because of this projection on a limited number of components, it is a useful technique for data with a lot of correlated variables and for which the number of variables exceeds the number of samples. The final results are linear regression models between the input and the output. The weights in these models can be used for interpretation of the connection between input (substrate composition) and output (biogas production).

An application of PLS is the calculation of the biochemical methane potential (BMP) of different substrates using composition variables. The BMP is the ultimate yield of biogas obtained in a batch digestion set-up [151]. Appels et al. [152] and Mottet et al. [153] both independently have developed non-dynamic models for waste-activated sludge with the former for mesophilic and the latter for thermophilic digestion, respectively. Appels et al. [154] measured the dry matter, organic dry matter, pH, total heavy metals content, sulphur, phosphorus, and some individual VFA ($\text{C}_2\text{--C}_7$). Additionally, the protein, carbohydrates and COD concentration of both the total sludge and the soluble phase were determined.

Subsequently, the insignificant variables were omitted to reduce the amount of experimental work for future validation and improve the performance of the model. The resulting model included the dry matter, organic dry matter, proteins, heavy metals, acetic acid, isobutyric acid, isovaleric acid and caproic acid. This model was based on 12 training samples and was validated on 2 new samples ($R^2 = 0.996$).

Mottet et al. [153] included the soluble organic carbon, proteins, carbohydrates, lipids, total VFA, sludge age, COD/TOC ratio, and the fractions of soluble, hemicellulose, cellulose and lignin in their model. The number of variables was subsequently reduced which resulted in a model that included the COD/TOC ratio, the soluble organic carbon, carbohydrates, lipids and proteins. The model was based on a 6-sample training set and a 4-sample validation set ($R^2 = 0.826$).

It is remarkable that both models were able to make good predictions, although they included different variables. This might have been the result of the different kinetics on going in thermophilic digestion. In general, however, it is not easy to draw comparisons between the two studies because different variables were included and the substrates used may have differed substantially.

Another application of PLS is the use of Near Infrared (NIR) to estimate the BMP. Lesteur et al. [154] developed a PLS model using NIR data of municipal and some specific waste types, and corresponding BMP measurements. Radiation in the NIR spectrum excites the vibrational and rotational energy levels in molecules, which results in unique absorbance spectral fingerprints for specific molecules. Traditionally, NIR spectra are used for organic composition estimations [155]. Instead of relating the spectra to the composition, however, Lesteur et al. [154] linked the spectra (1658–2500 nm) directly to the BMP. The results, based on 74 samples with 8 latent components, gave a Root Mean Square Error of Prediction (RMSEP) of 78 ml CH₄ g/VS and a $R^2 = 0.53$ based on 28 samples. This result can be further improved by analyzing more samples and constructing dedicated models for different specific types of waste. This technique has been commercialized by Ondalys® as Flash-BMP®.

In general, black-box models have several weaknesses compared to the descriptive and simplified models discussed previously. First, the interpretation of the resulting model is not straightforward. PCR or PLS result in regression models in which the coefficients indicate the importance of certain variables on the output, but do not give a clear view on the underlying mechanisms governing the process and leading to the obtained results. For ANN the number of layers and the weight given to the neurons form a complicated scheme in which it is hard to recognize any logic.

An additional problem, in addition to interpretability, is the degree of diversity within the data required to construct an accurate and robust model. In terms of the quantity of data, different sources disagree on guidelines, but at least 5–10 samples per parameter seems a desirable number [155]. For PLS, the necessary amount of data should relate to the number of independent, latent variables included in the model. A rule of thumb is 10 samples per latent variable, but this is probably under-estimation [156]. Care has to be taken that the origin of the data is aligned with the purpose of the data, e.g. data from widely differing conditions for a robust model, or from start-up situations for models that simulate start-up conditions. A final problem is that black-box models are prone to some degree of over-fitting and hence to simulating non-informative noise. This can be avoided by minimizing the number of

parameters used in the model, i.e. the number of orthogonal components in PLS and neurons and layers in ANN, but these should always be checked in a cross-validation.

The choice between the linearity (PLS) or non-linearity (ANN) is dependent on the intended purpose of the model. Non-linearity of the model arises when a feed-back regulations start to work. For static estimations (such as BMP), a linear approach (such as normal PLS) seems to be quite logical. For dynamic simulations of anaerobic digestions, that has plenty of feed-back loops, a non-linear approach, such as ANN, would be advisable.

5.2. Experience based models: fuzzy logic

Fuzzy logic modelling does not require a good understanding of the microbial processes occurring in the digestion mix or data set, but provides a good description of experience. Its power lies in the unique handling of data in fuzzy sets, in which data can exhibit partial degrees of membership to different classes. This is exemplified in five steps in Fig. 6: (1) An influent of a digester has 75 % low pH, 25% medium pH, 80% high COD and 20% low COD. (2) The degree of membership to each class is then related to the output using experience-based Boolean expressions. (3) These results are mapped in output membership functions, e.g. low and high biogas production. (4) The output functions are combined into one output function. (5) Finally, the function is de-fuzzified using, for instance, a centroid calculation that results in a precise single value of the output, e.g. the biogas production.

More recently the volumetric organic loading rate, total COD removal rate, influent alkalinity, and influent and effluent pH have been used as input variables for a discrete time model; each of them evaluated on 8 levels of membership functions which were further processed in the fuzzy-logic inference decision making module, with 134 logical rules [157]. The results are promising with accurate predictions of biogas production and methane content in steady-state conditions of an UASB digester. This interesting approach, however, in its current form is not very useful for making predictions as the effluent pH and COD removal rate are not known prior to digestion. However, this research successfully demonstrated the principle

A major issue with regards the application of fuzzy-logic based models is the quantification of experience in parameters, logical rules and membership functions. Erdirencelebi and Yalpir [158] proposed using an adaptive network fuzzy-inference system in which the membership functions were explicitly trained on data. Different schemes were examined with satisfactory predictions of pH, COD and VFA content of the effluent, based on the pH, COD and VFA content of the influent. The results, however, are quite ambiguous as the researchers also encountered the problem of under- and over-fitting, with regards to the number of connections made between the input and output parameters. Nevertheless, this approach shows potential as it objectifies the classification of data in different sets. This is especially true if different digestion situations are encountered, e.g. varying temperature or feed.

6. FUTURE RESEARCH NEEDS

Several innovations in the field of mathematical modeling of anaerobic digestion are most likely to, or should, attain a lot of attention in near future. First, the ADM1-framework will certainly be further modified with even more user specific application dependent modifications, with additional emphasis on the digestate properties. The estimation

methodology for ADM1 will mature: including full substrate characterization and resolving identifiability issues. Furthermore, new advances on the characterization of microbial community composition will pave the way to integrate these aspects in mathematical modeling. Finally, more specific black-box models will continually emerge.

6.1 ADM1

ADM1 was intended as a general framework that would allow further modifications. Its potential is illustrated by the modifications mentioned in Section 3.2.2. Up until now, however, the modifications generally are not focussed on digestate quality. Nevertheless, this is of great importance because these properties co-determine the economic viability of a substrate digest. Möller and Müller [159] calculated that for Germany, approximately 65.5 million cubic metres of digestate are produced annually. Most of this large amount of organic waste, if not contaminated with toxic components or large concentrations of heavy metals, is used as a fertilizer.

The quality of digestate (in dry or wet form) is mainly dependent on the availability of the nutrients: N, S and P in organic/inorganic and soluble/particulate form. This can be assured by further elaborating the reactions that affect the elemental mass balances: precipitation of sulphides, phosphates and struvite (MgNH_4PO_4).

Organic and inorganic phosphorous, both in soluble and particulate form are included in the CEIT-version, but precipitation of this element is not included. Inspiration could be found in the report of Batstone and Keller [105] who dealt with CaCO_3 precipitation. Sulphate reduction is already discussed by Fedorovich et al. [107], but is not regularly used.

It is worth mentioning that such a modification requires extra measurement of the cations, which can be done by inductively-coupled atomic emission spectrometry or mass spectrometry.

The characterisation of the substrate for an extensive model such as ADM1 is challenging. However, an approximation of composition can be determined following the procedures, as detailed by Kleerebezem and Van Loosdrecht [160] and Zaher et al. [161]. With both methods elemental composition of the waste mixture is first estimated using relatively simple measurements such as COD, total VFA, TKN, total inorganic nitrogen, total inorganic carbon, TOC, fixed solids and orthophosphate. Some of these measurements can be related to the elemental composition in a direct manner (TKN to N, total VFA to charge), using a balance of the valence electrons and the COD/TOC ratio [160, 161] or making a few assumptions of key parameters, e.g. COD of particulates originates mainly from carbohydrates [161]. Subsequently, the pooled elements (C, N, O, H, P and charge) are distributed over the different composition state variables, i.e. VFA, carbohydrates, proteins and lipids, of which the elemental composition is considered to be fixed. Kleerebezem and Van Loosdrecht [160] employed the balance of N and charge to determine the number of proteins and VFA. The lipid content was determined by comparing the overall oxidation state of the waste to the COD/TOC ratio. The remainder was taken to be represented by the carbohydrates.

The characterisation used by Zaher et al. [161], employs an extra balance for P and theoretical oxygen demand (ThOD) to determine the waste. Because this characterisation is implemented as a Continuity Based Interfacing Method (CBIM), described by Petersen matrices [162], it also yields the state variables of ADM1, with their specific elemental composition.

Using the same methodology, but specified to the particulate and inert state variables, Huete et al. [163] has set rules for the allocation of measurements in the ADM1-PWM framework.

A final issue is the identifiability of parameters for estimation purposes. In theory, the modelling procedure as outlined in Section 2 should be followed, starting with the analysis of the structural identifiability of the parameters. To our knowledge, the only analysis on structural identifiability was reported by Flotats et al. [164, 165]. They concluded that using batch tests with differing concentrations of proteins, valerate, amino acids and acetate, an univocal determination of the protein and valeric acid degradation parameters, together with the initial biomass concentration of the VFA degraders is possible. Also, the yield coefficients of protein, amino acid and valeric acid can be determined from the concentration profiles. If information on the identifiability is lacking, a minimum requirement would be to select the parameters on sensitivity basis such as reported by Lee et al. [16] or Girault et al. [166], although theoretically there is no guarantee that parameters that greatly influence the output, can be estimated with significant reliability. Due to the large number of parameters in the model, it is quite reasonable that the parameters can be fine-tuned to fit the data perfectly, while they are in fact not correct.

Indeed, the current literature is not very specific with regards the reliability of parameter or prediction estimations. Few, such as Batstone et al. [167] report the confidence intervals or regions of their estimates. Future work should, we feel, address the following question: how frequent and what should we measure to get a good estimate of parameters (and resulting) predictions? We hope that future research on validation of ADM1 will consider this recommendation.

The IWA Technical Report [4] provides, however, a qualitative indication of the variability and sensitivity of the parameters, indicating which parameters should be considered for identification. In addition it is common to determine the parameters based on prior assumptions of the rate-limiting steps, such as reported by Palatsi et al. [24] for LCFA kinetics and inhibition or Ramirez et al. [94] for disintegration and hydrolysis kinetics.

6.2. Microbial community data

In the models outlined previously, there has been no attempt to quantify specific microbial species present. Microorganisms are, if used as model variables, lumped together in their functional grouping, e.g. acidogenes, acetogenes, hydrogenotrophic methanogenes in ADM1 [4] and classified based according to their consumption or production of certain components. This classification is rather rudimentary because it completely neglects the enormous diversity of microorganisms (possibly) active in anaerobic digestion, as illustrated by Table 5, in which a selection of microbial community members is presented [5]. It also ignores the growing body of knowledge, largely based on genetic (DNA and RNA) finger-printing, regarding the presence and activity of key functional microbial populations.

The biomass of each population residing in anaerobic digestion culture, i.e. the microbial community composition, varies widely depending on digestion conditions, e.g. feed composition, digestion temperature, hydraulic retention time. These characteristic fluctuations are illustrated in several studies. For instance, Cirne et al. [168] identified the microbial communities in a two-stage batch digestion process of sugar beets and grass/clover. The main bacterial and archaeal groups responsible for hydrolysis were characterised. Moreover, clear

shifts in the microbial community composition were observed when hydrolysis step became the rate-limiting process. Other examples are provided by Delbès et al. [169], in which the microbial community composition and recovery was studied in response to a high dose of acetate and Regueiro et al. [23] who relate hydrolysis, acidogenic and methanogenic activity in different digesters to the presence of different phyla. Similarly, Shin et al. [170] reported that the community composition shifted continuously between four bacterial phyla and three archaeal orders, whilst digesting food waste-recycling wastewater.

The composition of microbial communities is not solely the result of the conditions to which it is exposed, but it is increasingly believed that it is the main parameter that defines the digestion performance. This is exemplified by the work of Werner et al. [171] who investigated the relationships between bacterial community composition and performance of several full-scale bioreactors. Over 5000 operational taxonomic units (OTU's, i.e. a surrogate for species) were detected within the different facilities and unique community structures were identified which exhibited a high degree of stability. Moreover, a stronger relation was detected between community structure and digestion performance than of the other operating conditions examined.

Developments on culture-independent molecular techniques, in recent years, have enabled improvements to be made with regards elucidation of microbial community composition and functional diversity. Examples of these techniques include polymerase chain reaction (PCR), DNA sequencing of PCR amplified genes, fluorescent *in situ* hybridisation (FISH), DNA stable isotope probing (DNA SIP), temperature and denaturing gradient gel electrophoresis (TGGE and DGGE), terminal restriction fragment length polymorphism (tRFLP), 454 pyrosequencing [172]. These techniques will be increasingly used in anaerobic digestion research, as has already occurred and have proven to be highly effective at providing a comprehensive report on the functional diversity of communities: FISH [168, 173], DGGE and real-time [170, 174], amplification of 16s ribosomal rRNA [168 - 175].

Inclusion of increasingly data rich information of microbial community composition, could drastically improve model performance. This is exemplified by Ramirez et al. [176] who adjusted ADM1 in order to take into account microbial community diversity. Their work resulted in an improvement of predictive performance when the kinetic parameters were replaced by a set of 10 stochastically chosen kinetic parameters, each representing a separate microbial species. However, in conjunction with the previously mentioned measuring techniques, it will become possible to explicitly denominate the functionally active microbial populations and examine their kinetics. This has already been demonstrated by Vavilin et al. [177] based on data from Li et al. [178] who examined *Methanosarcina* sp. with FISH and NanoSIMS (nano secondary ion mass spectrometry).

6.3. Black –box models

In general, any phenomenon that shows a relationship with certain composition variables, be it a direct one or not, can be modelled using a black-box approach. The main requirements are the existence of this latent relationship, the collection of sufficient and informative data, and a weak or non-existent feed-back relationship between the input and output variables. It is expected that black-box models will be used and/or further extended to address several key process variables, namely BMP determinations and predicting foaming.

Because of the ever increasing interest in anaerobic digestion as process itself and as a sustainable energy source, increasing numbers of organisations want to perform BMP assays on specific substrate using specific anaerobic biomass. However, BMP such as described by Angelidaki et al. [151] take up to 50 days to obtain the final results. In the future, databases such as used by Appels et al. [152], Mottet et al. [153] and Lesteur [154] will be further extended and diversified to provide substrate-specific models and commercialised. Another example of the latter is given by the test-kit Envital[®], developed by Envulure[®], which relates the BMP to activity measurements by fluorescence of anaerobic bacteria on the analysed substrate.

Foaming of sludge is a common problem for activated sludge systems. This problem, however, is also encountered in anaerobic sludge digestion systems fed with activated sludge and causes an inefficient gas recovery, flotation of the solids, the creation of dead zones and interference with the digester devices, such as sensors and mixers. The causes of foaming are attributed to several factors: the occurrence of certain filamentous microorganisms in the fed sludge, surface-active agents such as lipids, VFA's, detergents, proteins, inorganic matter and the temperature and rate of mixing of the digester [179]. A mechanistically inspired model that predicts foaming phenomena would be exceedingly complex as it needs to contain information on the microbial structure of the incoming and residing sludge and the spatial description of the digester, using partial differential equations. Therefore, black-box approaches are more appropriate to give a quantitative evaluation of the risk of foaming. Dalmau et al. [180] have previously reported a fuzzy-decision theory model that predicts the foaming risk based on the organic loading rate and a factor that describes the risk of foaming of the substrate in its aerobic environment. The latter is based on operation conditions such as the substrate-to-microorganism ratio, the sludge retention time and the dissolved oxygen. However, it is more logical to relate the foaming to direct causes of the sludge: the composition and occurrence of filamentous microorganisms in the influent and/or digester content. The latest innovations in microscopy and image processing make such an automatic, and ideally real time, detection and evaluation of the structure of the microorganisms possible, as exemplified by the evaluation of the sludge settling ability by analysing the microscopic structure, reported by Jenné et al. [181] and Mesquita et al. [182].

CONCLUSIONS

Modelling of anaerobic digestion has evolved drastically: starting from very simplified models that consider digestion as a fermentation process from sugars, to the advanced and extended models such as ADM1. The latter can be thought of as a conjunction of 'knowledge' on anaerobic digestion modelling. It comes in three versions and many adaptations have been made to address certain caveats or specific digestion situations. It is mainly used as a benchmark, either stand-alone or in a plant-wide model, which requires interfacing.

Additionally, more parsimonious models are nevertheless used for control purposes. The proposed models use easy-to-measure variables and their simplicity makes a whole myriad of control actions possible, with or without state estimation.

Although major interest is given to the development of mechanistically inspired models, they are not the only prodigy of modelling efforts. Black-box models, based either on statistical methods or heuristical information give elegant solutions to estimation problems, on the

precondition that sufficient data is available. The models mentioned in this review are suited for the conditions mentioned in their respective references, but we believe that the approaches can be valuable for user-specific conditions, i.e. other data sets.

It is believed that future developments will primarily focus on the biological aspect of modelling: mathematically relating the performance of a digestion to microbial diversity and activity.

Acknowledgements

The authors would like to thank the Agency for Innovation by Science and Technology in Flanders (IWT/100196) and the Research Council of the KU Leuven (PDMK/10/121) for the financial support. This work was supported in part by Project KP/09/005 (SCORES4CHEM Knowledge Platform) and Project KP/10/006 (AOptimise Knowledge Platform) of the Industrial Research Council of the KU Leuven, Project PFV/10/002 Centre of Excellence OPTEC-Optimization in Engineering and the Belgian Program on Interuniversity Poles of Attraction initiated by the Belgian Federal Science Policy Office. Jan Van Impe holds the chair Safety Engineering sponsored by the Belgian chemistry and life science federation essenscia.

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Abbreviations:

1 st	1st order kinetics
AA	Amino acids
AC	Acetate
ACET	Acetogenesis kinetics
ACET METH	Acetogenotrophic methanogenesis
ACID	Acidogenesis kinetics
AE	Algebraic equations
ADM1	Anaerobic Digestion Model No. 1
ANN	Artificial Neural Networks
ASM1/2/3	Activated Sludge Model No. 1/2/3
BMP	Biochemical methane potential
BSM2	Benchmark simulation model no. 2
C2	Acetic acid
C3	Propionic acid
C4	Butyric acid
C5	Valeric acid
C6	Caproic acid
C	Contois kinetics
CBIM	Continuity-base interfacing method
CD	Cell death
CH	Carbohydrates
COD	Chemical oxygen demand (g O ₂ /L)
COMP	Intermediate components
CSTR	Continuous stirred tank reactor
DNA SIP	DNA stable isotope probing
EBK	Equilibrium-based kinetics
F	Full scale
FA	Fatty acids
FISH	Fluorescent in situ hybridization
FOG	Fats, oils and greases
H	Haldane kinetics
Hva	Haldane kinetics with unionized volatile fatty acid inhibition
HYD METH	Hydrogenotrophic methanogenesis
HYDR	Hydrolysis kinetics
IWA	International water association
LI	Lipids
LCFA	Long-chain fatty acids
L-G	Liquid-gas mass transfer
M	Monod kinetics
METH	Methanogenesis
NA	Nucleic acids
NanoSIMS	Nano secondary ion mass spectrometry
ODE	Ordinary differential equations
OTU	Operational taxonomic unit
P	Pilot scale
PA	Propionate
PCR	Principal component regression
PID	Proportional-integral-derivative

PLS	Partial least squares
PWM	Plant-wide modeling
PROT	Proteins
RMSE	Root mean square error of prediction
SBK	Surface-based kinetics
SVM	Support Vector Machines
TA	Total alkalinity
TGGE	Temperature and denaturing gradient
ThOD	Theoretical oxygen demand
tRLFP	Terminal restriction fragment length polymorphism
tVFA	Ionized and unionized VFA
VSS	Volatile suspended solids
UASB	Upflow anaerobic sludge bed
VFA	Volatile fatty acids
WWTP	Wastewater treatment plant

Table 1 Mechanistically inspired models: summary of the most cited models with (i) the specifically included intermediate components (COMP) , (ii) hydrolysis kinetics (HYDR), (iii) acidogenesis kinetics (ACID), (iv) acetogenesis kinetics (ACET), either of VFA (VFA ACET) or of LCFA (LCFA ACET), (v) methanogenesis kinetics (METH), either acetogenotrophic (ACET METH) or hydrogenotrophic (HYD METH) (vi) the inclusion of cell death (CD), (vii) Liquid-Gas mass-transfer (L-G), (viii) calculation of pH based on ion balance (pH), (vii) specific characteristics, (viii) field of application and (ix) reported scale of applications (L = Lab Scale (digester volume $V < 15$ L), P = Pilot Scale ($15L < V < 1000L$), F = Full-Scale ($V > 1m^3$)). If no reference is given, the application is found in the original paper. Inhibition or regulations of the kinetics are denoted by the parameters between brackets. Other abbreviations: Acetic acid (C_2), Propionic Acid (C_3), Butyric Acid (C_4), Valeric Acid (C_5), Caproic Acid (C_6), Monod Kinetics (M), 1st order kinetics (1st), Haldane kinetics (H), Haldane with unionized volatile fatty acid inhibition (H_{VA}), Surface-based kinetics (SBK), Contois kinetics (C), Equilibrium-based kinetics (EBK), Acetate (AC), Propionate (PA), Carbohydrates (CH), Proteins (PROT), Fatty Acids (FA), Nucleic Acids (NA), Lipids (LI), ionized and unionized VFA (tVFA).

Authors	COMP	HYDR	ACID	ACET		METH		CD	pH	L-G	NH ₃	Specific characteristics	Applic ation	Scale
				VFA ACET	LCFA ACET	ACET METH	HYD METH							
Andrews and Pearson[26]	C_2	-	M	-	-	M	-	X	-	-	-	Yield and kinetics estimated from steady – state condition	Dissol ved organi cs	L
Andrews [27]	C_2	-	-	-	-	H_{VA}	-	-	-	-	-	METH rate limiting	Dissol ved organi cs	L
Andrews and Graef [28]	C_2	-	-	-	-	H_{VA}	-	X	X	X	-	METH rate-limiting	Dissol ved organi cs	L
Graef and Andrews [59]	C_2	-	-	-	-	H_{VA}	-	X	X	X	-	METH rate-limiting	Dissol ved organi cs	L, P [60]
Hill and Barth [52]	-	H_{VA}	H_{VA}	-	-	$H_{VA}(NH_3)$	-	X	X	-	-	-	Anima l waste and	P [61]

												manur e	
Eastman and Ferguson [35]	C ₂	1st	-	-	M		X	-	-	-	HYDR rate- limiting. No distinction in fermentation products, i.e. the final product is total COD originating from acids, CH ₄ , CO ₂ , proteins...	Particu late	L
Kleinstreuer and Poweigha [62]	C ₂	-	-	H _{VA}	H _{VA}		X	X	-	-	-	Dissol ved organi cs	L
Hill, [63] Hill et al. [64]	C ₂ -C ₄	-	H _{VA}	H _{VA}	H _{VA}	H _{VA}	X(tV FA)	-	-	-	-	Anima l waste and manur e	L, P
Mosey [32]	C ₂ -C ₄	-	M	M(H ₂)	M	M (NH ₃ , pH)	X	-	-	X	The acidogenesis stage follows the Embden- Meyerhof pathway Equations based on NADH balances	Glucos e	-
Moletta et al. [65]	C ₂	-	growth: H _{VA} consumptio	-	growth: H _{VA} consumption:		X	-	-	-	Different expressions for	Dissol ved	L

			n: M		M(AC _{unionized})						consumption and associated biomass growth	organi cs	
Denac et al. [29]	C ₂ -C ₄	-	M	M	M		X	-	X	-	Biofilm diffusion model, but with similar results to a homogenous model	Dissol ved organi cs	L
Bastin and Dochain [66]	-	Undefined M, H or C [67]					X	-	-	-	Components are lumped variables expressed in terms of COD	Particu late	L
Costello et al. [44]	C ₂ -C ₄ Lactic acid CH PROT, LI [68]	- 4/3 st order (enzyme concentrat ion) [68]	M(pH, H ₂ , AC)	M(pH, H ₂ , AC)	M(pH)	M(pH)	X	X	X	-	Acid production stoichiometry is hydrogen regulated and inhibited Hydrolysis by soluble enzymes produced by the bacterial group that utilizes the associated substrate [68]	Waste water	P [45], F [68]
Shimizu et al. [50]	C ₂ -C ₆ CH NA LI	1st	1st	1st	1st	1st	X	-	-	-	Separate decomposition kinetics of different VFA Nucleic acid degradation	Sludge	L

Kalyuzhnyi and Davlyatshina [33], Kalyuzhnyi [34]	C ₂ - C ₄	-	M(pH, H ₂)	M(pH, H ₂) Ethanol acetogenes: M(pH, H ₂)	M(pH, H ₂)		X	-	-	-	Ethanol generation and degradation pathway	Glucose	L
Bryers [69]	C ₂ -C ₃ FA	1st	M	M	M	M	X	X	X	-	Particulate substrate is lumped together	Particulate	L
Kaluzhnyi <i>et al.</i> [56]	C ₂ -C ₅	1 st (pH)	EBK(pH)	EBK(pH)	EBK(pH)	EBK(pH)	X	X	X	X	Mass transfer between seed and substrate particles	Solid waste	-
Batstone et al. [46,47]	C ₂ -C ₅ Lactic acid CH PROT LI	4/3rd order with non-competitive enzyme regulation	M(pH, H ₂)	M(pH)	M(pH)	M(pH)	X	X	X	X	Hydrolysis by soluble enzymes produced by the bacterial group that utilizes the associated substrate Acid production stoichiometry is hydrogen regulated and inhibited	Waste water	F
Pavlostathis and Gosset [70]	C ₂	1st	M	-	M		X	X	-	-	Viable cells die/lyse (1st order) into an intermediate particulate requiring hydrolysis	Sludge	L
Siegrist et al. [71]	C ₂ -C ₄ CH PROT	1st	M(pH)	M(pH, H ₂ , AC)	M	M(pH)	X	X	X	-	CO ₂ /HCO ₃ ⁻ transfer is an 1 st order process	Sludge	P

	LI													
Siegrist et al. [49]	C ₂ -C ₃ CH PROT LI	1st	M(pH)	M(pH, H ₂ , NH ₃ , AC)	M(pH, H ₂ , AC)	M(pH, NH ₃)	M(pH)	X	X	X	X	Differences in decay rates CO ₂ /HCO ₃ ⁻ , NH ₃ /NH ₄ ⁺ and VFA acidification: 1 st order process	Sludge	F [72]
Sötemann et al. [73]	-	1st order, 1 st order (ACID biomass), M or C	-	-		-		-	-	-	-	Hydrolysis rate-limiting Steady-state biogas production and ACID biomass 4 hydrolysis/acid ogenesis kinetics considered	Sludge	L, F [74]
Hobson [42]	C ₂	SBK	M	-		M(NH ₃)	M(NH ₃)	-	-	-	X	Substrate specified in size and surface to materials. Inhibitory effects of ammonia and high input solids concentrations	Animal waste and manure Fibrous waste	L

Angelidaki <i>et al.</i> [53,54]	C ₂ -C ₄ CH LI [54]	1 st (tVFA)	M	M(AC, pH)		M(NH ₃ , pH)	-	X	X	X	X	Controlled by the pH-VFA-NH ₃ interaction on the acetogens and the methanogens. LCFA degradation [54]	Animal waste and manure	L[75]
Vavilin et al. [76] (“METHANE”)	C ₂ -C ₃	Limited 1st or M		M(NH ₃ , pH, PA)		M(NH ₃ , pH, H ₂ S, PA)		X	X	X	X	SO ₄ ²⁻ reduction to H ₂ S by consumption of C ₂ and C ₃ (M) Phosphorous (PO ₄ ³⁻) Non-degradable solids Minerals (Ca ²⁺ ,Na ⁺)	Various	L [77-79]
Kiely et al. [80]	-		H _{VA}	-		H (NH ₃)		X	X	X	X	-	Animal waste and manure	L
Angelidaki et al. [58]	C ₂ -C ₅ CH PROT LI LCFA	1 st (tVFA)	M(NH ₃ , pH, LCFA) lipolytic: M(NH ₃ , pH, LCFA)	M(NH ₃ , pH, AC)	H(NH ₃ pH)	H(NH ₃ , LCFA)		X	X	X	X	Monod type ammonia-N co-substrate dependency glycerol degrading lipolytic	Various	L, F

												bacteria		
Bernard et al. [20]	-	M		-		H		X	X	X	-	Components are lumped variables expressed in terms of COD	Waste water	P see Section 4
Batstone et al. (ADM1) [4]	C ₂ -C ₅ LCFA CH PROT LI	1 st	M(pH, limiting Nitrogen)	M(pH, limiting Nitrogen, H ₂)	M(pH, limiting Nitrogen)	M(pH, limiting Nitrogen, NH ₃)	X	X	X	X	Degradation step before hydrolysis Modifications reported in Section 3.2.2	Variou s	see Section 3.2	

Table 2 Modifications and applications of ADM1.

Authors	Extension/adaptation of ADM1	Application
Batstone and Keller [105]	Precipitation of CaCO_3	Various
Batstone et al. [106]	Acetogenesis of isovalerate	Protein rich substrate
Fedorovich et al. [107]	Reduction of sulphate to H_2S by oxidising propionate, acetate, butyrate/valerate and hydrogen oxidising biomass	Sulphate rich substrate
de Gracia et al. [86] and Wett et al. [108]	Distinction between particulate and dead biomass Inclusion of inert decay products	Various
Parker et al.[109]	Methoxylated aromatic compounds, methyl mercaptan, dimethylsulphide conversion into hydrogen sulphide (microbial) Metal sulphide precipitation	Sulphur rich substrate
Tugtas et al. [110]	Oxidation of nitrate to nitrite, nitric oxide, nitrous oxide and nitrogen by propionate and butyrate/valerate degraders. Non-competitive inhibition by nitrogen oxides	Various
Rodríguez et al. [100]	pH and hydrogen dependence of carbohydrate fermentation stoichiometry	Various
Peiris et al. [96]	Lactate and ethanol as intermediates	Bio-hydrogen production
Fountoulakis et al. [111]	Degradation of di-ethylhexyl phthalate (sorption-desorption based kinetics)	Sludge
Kleerebezem and van Loosdrecht [99]	Powered expression for hydrogen inhibition of acetogenesis and hydrogen consumption in methanogenesis	Various
Zaher et al. [97]	Cyanide hydrolysis and uptake. Cyanide inhibition of acetogenes. Classification into cyanide resistant and non-resistant methanogenes	Cyanide containing wastes. Can be generalised to other toxics
Shimada et al.[112]	Storage of reserve polymers by microorganisms	Digestion with rapid changing conditions
Myint et al.[113]	Particulate and soluble cellulose and hemicellulose Hydrolysis kinetics considering surface colonization and biodegradation	Particulate containing cellulose and hemicellulose
Ramirez et al. [94]	Contois kinetics for disintegration and hydrolysis, Hill function for ammonia inhibition	Sludge
Yasui et al. [114]	Substrate classification on degradation properties	Sludge
Penumathsa et al. [95]	Variable stoichiometry according to Rodríguez et al. [100] Lactate degradation (microbial)	Bio-hydrogen production
Fezzani and Ben Cheick [89]	Inhibition of acetogenic methanogenesis by total VFA	Various
Fezzani and Ben Cheick [115]	Particulate and soluble phenols. Degradation by hydrolysis (1st) and acidogenesis (Haldane)	Phenol rich substrate
Palatsi et al. [24]	LCFA uptake (Haldane). LCFA inhibition of acetogenes and hydrogenotrophic methanogens (non competitive) or via adsorption-based inhibition	Lipid rich substrate
Bollon et al. [116]	Lumping of disintegration, hydrolysis and acidogenesis	Dry digestion
Mairet et al. [92]	Contois kinetics for hydrolysis	Particulate waste
Esposito et al. [117]	Surface-based kinetics for hydrolysis	Particulate waste
Hierholtzer and Akunna [98]	Sodium as an extra variable. Non-competitive inhibition of sodium on acetoclastic methanogens	Sodium rich substrate

Table 3 Control approaches based on the model Bastin and Dochain [66].

Authors	Control type	Description
Stoyanov and Simeonov [130]	Robust compensator control	Step-wise set points asymptotic tracking and external disturbances rejection
Zlateva [129]	Sliding-mode control	Discontinuous control signal determined by switching functions. Invariant to parameter uncertainties and external disturbances
Stoyanov [131]	Robust multiple-input; multiple-output control	The dilution and feed concentration consist of terms that ensure nominal system stability and to compensate parameter uncertainty
Simeonov and Stoyanov [132]	Dynamic compensator control	Control of dilution by a combination of an internal model that ensures set-point tracking and a stabilisation part

Table 4 Control approaches based on the model of Bernard et al. [19]

Authors	Control type	Description
Bernard et al. [20]	Adaptive control	A mass-balance based controller that gives linear closed loop dynamics. The model parameters only need to be approximated.
Mailleret et al. [135]	Robust non-linear control	A mass-balance based controller that gives linear closed loop dynamics. The yield coefficients need to be known. The inputs of the process do not need to be measured.
Alcaraz-González et al. [136]	Interval based non-linear control	Combination of a soft-sensor (interval observer) and a robust feedback control. The model parameters and inputs are only approximately known, i.e. the interval they span. The controlled variable is kept in a certain region, rather than at a certain fixed set-point.
Grogard and Bernard [137]	Saturated proportional controller	A proportional controller that ensures; Attraction to a region of the state space, rather than a set-point. It requires measurement of the total COD value (S_1 and S_2).
Méndez-Acosta et al. [138]	Robust control	Multiple-input; multiple-output linearising control volatile fatty acids (VFA) and total alkalinity (TA), by controlling the influent flow rate and the addition of an alkali solution. The process kinetics and variations in the influent composition is estimated using a soft-sensor (extended Luenberger observer).

Table 5 Genera active in different stages of anaerobic digestion [5].

Active in Hydrolysis, acidogenesis, acetogenesis and methanogenesis
Acetobacterium, Eubacterium
Ruminococcus, Paenibacillus, Clostridium (mostly in acidogenic stage)
Active in hydrolysis stage
Bacteroides, Lactobacillus, Propioni-bacterium, Sphingomonas, Sporobacterium, Megasphaera, Bifidobacterium
Active in acidogenic stage
Ruminococcus, Paenibacillus, Clostridium
Active in acetogenic stage
Desulfovibrio, Aminobacterium, Acidaminococcus
Active in methanogenic stage
Methanobrevibacter, Methanobacterium, Methanosphaera, Methanothermobacter, Methanothermus, Methanococcus, Methanothermococcus, Methanomicrobium, Methanolacinia, Methanogenium, Methanoculleus, Methanoplanus, Methanofollis, Methanocalculus, Methanocorpusculum, Methanospirillum, Methanosarcina, Methanolobus, Methanococcoides, Methanohalophilus, Methanosalsus, Methanohalobium, Halomethanococcus, Methanosaeta

Figures

Fig. 1 Schematic overview of the anaerobic digestion process.

Fig. 2 Schematic overview of the dynamic modelling procedure [13,14].

Fig. 3 The reaction paths described in ADM1 [4], with the following microbial groups: (1) sugar degraders, (2) amino acid degraders, (3) LCFA degraders, (4) propionic acid degraders, (5) butyric and valeric acid degraders, (6) acetoclastic methanogens, and (7) hydrogenotrophic methanogens.

Fig. 4 Benchmark Simulation Model No. 2 [118].

Fig. 5 ASM1/ADM1 and ADM1/ASM1 interfacing in 6 and 4 steps, respectively. ASM1 variables are in white and ADM1 in grey. Solid lines depict the allocation of a variable to a pool or another variable. Dotted lines depict allocations of the remainder of a variable after a first allocation [120].

Fig. 6 Fuzzy logic modelling scheme for predicting biogas production.