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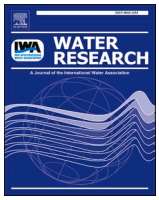

Review

Modifications to the anaerobic digestion model no. 1 (ADM1) for enhanced understanding and application of the anaerobic treatment processes – A comprehensive review

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ABSTRACT

Anaerobic digestion (AD) is a promising method for the recovery of resources and energy from organic wastes. Correspondingly, AD modelling has also been developed in recent years. The International Water Association (IWA) Anaerobic Digestion Model No. 1 (ADM1) is currently the most commonly used structured AD model. However, as substrates become more complex and our understanding of the AD mechanism grows, both systematic and specific modifications have been applied to the ADM1. Modified models have provided a diverse range of application besides AD processes, such as fermentation and biogas upgrading processes. This paper reviews research on the modification of the ADM1, with a particular focus on processes, kinetics, stoichiometry and parameters, which are the major elements of the model. The paper begins with a brief introduction to the ADM1, followed by a summary of modifications, including extensions to the model structure, modifications to kinetics (including inhibition functions) and stoichiometry, as well as simplifications to the model. The paper also covers kinetic parameter estimation and validation of the model, as well as practical applications of the model to a variety of scenarios. The review highlights the need for improvements in simulating AD and biogas upgrading processes, as well as the lack of full-scale applications to other substrates besides sludge (such as food waste and agricultural waste). Future research directions are suggested for model development based on detailed understanding of the anaerobic treatment mechanisms, and the need to recover of valuable products.

1. Introduction

Anaerobic digestion (AD) is a biological process that converts biodegradable organic wastes into biogas, making it a well-established technology for the treatment of organic wastes and a proven method for producing renewable and clean energy (Chen et al., 2016, 2022). The process utilizes a variety of generalist and specialist clades of archaea and bacteria to generate and consume intermediate compounds, including organic acids. Inappropriate operating conditions can lead to process instability and significant reduction in methane production. Therefore, predicting and regulating AD processes is crucial for optimizing system design and operation. Mathematical modelling is an important approach for predicting biogas production and optimizing the AD system. Many mathematical models, including unstructured (not considering intermediates) and structured (considering intermediates) models, have been developed to monitor and predict AD processes (Batstone et al., 2002). Unstructured models generally consider hydrolysis to be rate limiting (i.e., single step), and include first order (Dennehy et al., 2016; Kafle and Chen, 2016), Monod (Lokshina et al., 2001), Contois (Karim et al., 2007) and modified Gompertz (Pan et al., 2019; Xie et al., 2011; Zou et al., 2018) models. These have been widely used because of their simple structure, identifiability, and limited number of parameters. However, because hydrolysis only is considered, they cannot predict major failure modes, such as acidification, nor important outputs, such as pH, volatile fatty acids (VFAs) concentrations, and methane content.

The International Water Association (IWA) Anaerobic Digestion Model No. 1 (ADM1) is a commonly used structured model, which was

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developed by an IWA task group (Batstone et al., 2002). The ADM1 is based on the "four-stage theory of anaerobic digestion" (i.e. hydrolysis, acidogenesis, acetogenesis and methanogenesis) (Zeikus et al., 1985), which is considered a moderate approach to the inclusion of relevant processes to simulate the change of substrates, intermediates, final products and major microbial clades in AD (Yang et al., 2020). The ADM1 was informed by a number of precedent models (Batstone et al., 2002). In particular, because the concentrations of important intermediates, such as lactic acid and ethanol, are normally low in anaerobic reactors, these compounds are neglected in the original ADM1. With broader application, development of AD technologies, and application to specific wastewaters, the ADM1 can fail to effectively describe key mechanisms and intermediates (Fedorovich et al., 2003). Moreover, difficulties in the characterization for a broad array of wastewater types have been highlighted by publication of a generalized model. Importantly, phosphorus (P), iron (Fe) and sulfur (S) transformations were specifically excluded despite being recognized as important due to a lack of precedent research at the time of publication (Batstone et al., 2002). This has resulted in modification of the ADM1 being the focus of publications over the past two decades. Parker (2005) summarized the application of the ADM1 to advanced AD processes. Batstone et al. (2006a) reviewed extensions to the ADM1 in the early years (2002–2005). They focused on the model extensions, such as sulfate reduction, and simple phosphorus balances, largely reiterating previous gaps. Later, Batstone et al. (2015) provided a further summary, mainly the improvement of the ADM1 in plant-wide modelling, identifying developments in the linked phosphorus-sulfur-iron processes across the cycle, and proposing removal of composite particulates concept (X_C). These reviews have largely focused on extensions, rather than model core, and are somewhat dated. A further review of key elements of the model, such as major processes, kinetic expressions (especially the inhibition functions), stoichiometry and parameters, is still lacking in all aspects.

The objective of this study is to summarize modifications to the major elements of the ADM1 and approaches to model calibration/validation, as well as practical application of the model. The review begins with introducing the original ADM1 and then investigates modification to the ADM1, including extensions to the model structure, modifications of the stoichiometry and the kinetic expressions including inhibition functions, as well as simplification to the model in some cases. Approaches to model calibration/validation, along with the ranges of reported model parameters, are discussed, and practical applications of ADM1 are summarized. Finally, future research directions, perspectives and challenges are outlined. This review is expected to provide a comprehensive understanding of the ADM1 and serve as a foundation for the subsequent model development, helping in better prediction and regulation of performances of the AD or other processes.

2. A brief description of the original ADM1

The ADM1 is a structured model describing the biochemical and physicochemical processes of AD. The model is described in considerable detail in the relevant scientific report (Batstone et al., 2002). Components, processes, stoichiometric coefficients, kinetic expressions and the relevant parameters are the major elements of the ADM1, and all these elements are involved in a Petersen matrix to realize the quantitative description of the AD process (Batstone et al., 2002).

As for most mechanistic biochemical models, intensive state variables are utilized, with soluble components (expressed as S in the model) and particulate components (expressed as X in the model) including microbial biomass, separated by functional clades, and substrate particulates. These are represented by state variables, with biochemical and chemical processes acting as source/sink elements in the general mass balance. Biochemical processes of AD in the model include five steps: disintegration, hydrolysis, acidogenesis, acetogenesis, and methanogenesis. An overview of the components and bioconversion processes that are addressed by the model is presented in Fig. 1. The ADM1 as originally published proposed a two-step solubilization process, with composite particulates (X_C) being "disintegrated" to particulate proteins (X_{pr}), carbohydrates (X_{ch}), lipids (X_{li}), and inert substances (X_i and S_i), and the degradable disintegration products then being "hydrolysed" to amino acids (S_{aa}), sugars (S_{su}), and long-chain fatty acids (LCFAs, S_{fa} in the model), respectively. In the following acidogenesis process, sugars and amino acids are fermented into VFAs, hydrogen and carbon dioxide by different degraders, and LCFAs are oxidized to produce acetate and hydrogen. Furthermore, propionic acid (S_{pro}), butyric acid (S_{bu}) and valeric acid (S_{va}) are anaerobically converted into acetate (S_{ac}), carbon dioxide (S_{co2}) and hydrogen (S_{h2}). The last step of methanogenesis includes aceticlastic methanogenesis where methane is produced by cleavage of acetate, and hydrogenotrophic methanogenesis, in which carbon dioxide is converted by hydrogen-utilizing methanogenic bacteria into methane (S_{ch4}). Biomass growth is implicit in substrate uptake, and linked by a yield coefficient. Decayed biomass returns to the fraction of complex organics and undergoes disintegration and hydrolysis. In addition to the organic species, inorganic carbon (S_{IC}) and nitrogenous species (S_{IN}) are included as acid-base active compounds, and used as elemental balance closures. Chemical oxygen demand (COD), is used a principal unit, with the zero-COD nitrogenous species and inorganic carbon species described in terms of their molar concentrations.

Substrate conversion rates are expressed as a number of process kinetics. The disintegration and hydrolysis of complex organic matters which are extracellular processes are described as first-order kinetics based on the substrate concentration. Decay of biomass is also presented by first-order kinetics. This function is an empirical expression that is assumed to reflect the cumulative effects of extracellular processes and ignore microbial effects (Mottet et al., 2013). Monod-type kinetic expressions, as shown in Fig. 1, are used as the basis for all intracellular biochemical processes (acidogenesis, acetogenesis and methanogenesis).

Intracellular conversion processes can be inhibited by inappropriate pH (Latif et al., 2017) or the accumulation of intermediate products, such as inorganic nitrogen, free ammonia (Astals et al., 2018; Rajagopal et al., 2013; Zheng et al., 2021), molecular hydrogen (Cazier et al., 2019) et al. The effects of these inhibitions are quantified as inhibition functions (I) and expressed in the kinetics as follow:

$$\rho_j = \rho_{max} \cdot I_1 I_2 I_3 \tag{1}$$

where ρ_{max} is the Monod-type kinetic equation without inhibitions and I_i are inhibition functions.

Stoichiometric coefficients are quantitative description of the formation and conversion of components in the AD, which ensure the mass balance of elements in the process reactions and imply the microbial growth in the corresponding uptake processes.

The physicochemical processes in ADM1 involve six acid/base equilibria in association with pH solved by a charge balance approach and three gas-liquid transfer processes for CH_4, CO_2, and H_2.

Acid-base reactions relating to physicochemical reactions in the liquid phase can be implemented as differential-algebraic equations (DAE) or differential equations (DE). If implemented as a DAE system, the acid/base pairs are normally lumped as a combined dynamic state variable, and the concentration of individual acid or base is calculated from the following acid-base equilibria equation:

$$S_{i^-} - \frac{K_a S_i}{K_a + S_{H^+}} = 0 \tag{2}$$

where K_a and S_{H^+} denote the acid-base equilibrium constant and the variable for hydrogen ion concentration, respectively. pH is determined by the proton concentration, which is determined directly by solution of the implicit algebraic set as noted above.

If the liquid phase equations are implemented as DE, acid-base transfer would be described by an additional dynamic rate equation shown as follow:

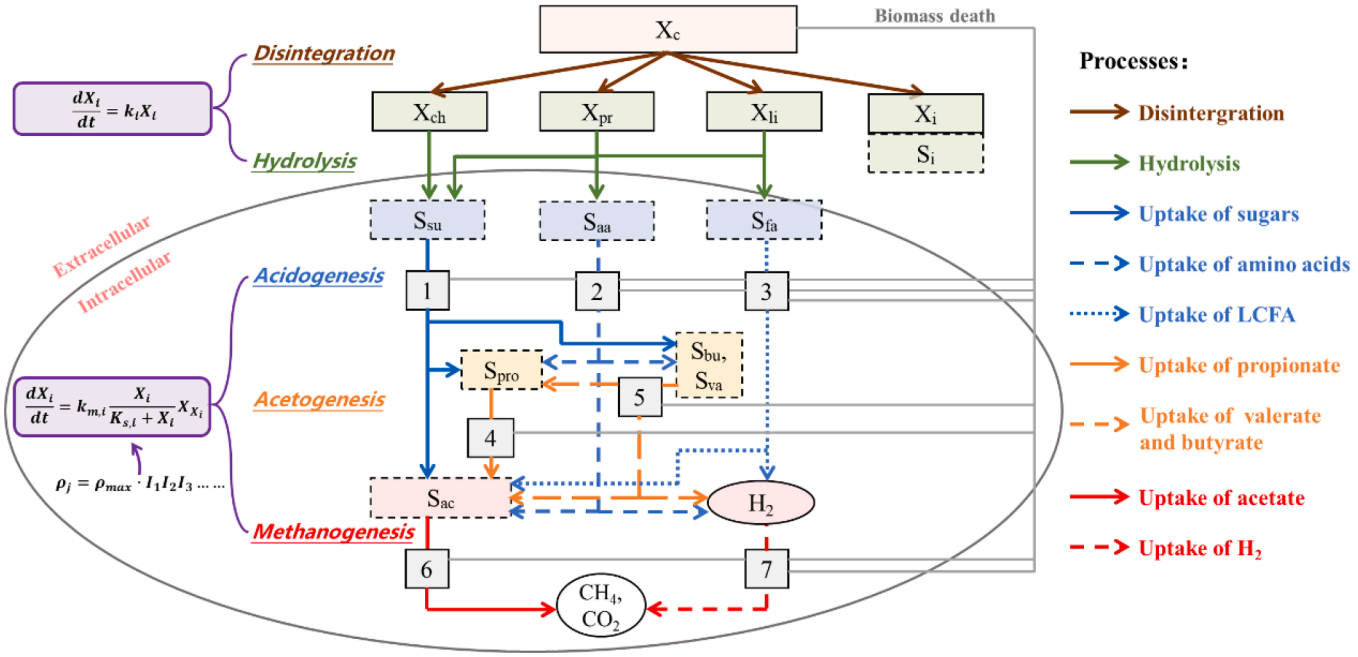

Fig. 1. The conceptual model for ADM1: (1) sugar degraders (X_{su}), (2) amino acid degraders (X_{aa}), (3) LCFAs degraders (X_{fa}), (4) propionate degraders (X_{pro}), (5) butyrate and valerate degraders (X_{c4}), (6) acetate degraders (X_{ac}), and (7) hydrogen degraders (X_{h2}).

$$\rho_{A|B,Hi} = k_{A|B}\left(S_{liq,H}S_{liq,i} - K_{a,Hi}S_{liq,Hi}\right) \quad (3)$$

where $k_{A|B}$ is the rate coefficient for the base to acid reaction, $S_{liq,H}$, $S_{liq,i}$ and $S_{liq,Hi}$ are concentration of hydrogen ion, acid ion and acid, respectively, and $K_{a,Hi}$ are the acid association and dissociation constant.

During the dynamic AD processes, gaseous components (CH_4, CO_2, H_2) become supersaturated in the liquid phase and transfer into the gas phase (Zhang et al., 2015), which is described by the gas transfer rate equation shown as follows:

$$\rho_{T,j} = k_L a_j\left(S_{liq,j} - K_{H,j}P_{gas,j}\right) \quad (4)$$

where $S_{liq,j}$ is the dynamic state variable for soluble gas, $P_{gas,j}$ is the pressure of gas, $k_L a_j$ is the gas-liquid transfer coefficient and $K_{H,j}$ is the Henry's law coefficient. Gas-liquid transfer is determined by two film (liquid film and gas film) controlled mass transfer (liquid film controlled).

The original ADM1 presents a generic structure model initially devised for AD of sewage sludge. However, this model exhibits constrains in both its biochemical and physicochemical parts. In some biochemical processes, specific components and inhibitions were omitted from the model due to their low concentrations or unfavourable conditions in AD of sewage sludge. However, these exclusions can introduce biases into model simulations. For example, in the fermentation of carbohydrate-rich substrate, the accumulation of lactate and ethanol (which were not accounted for in the original model) can exert significant influence on both acidogenesis and methanogenesis. Consequently, this oversight can lead to inaccurate simulations of intermediates, such as VFAs, and ultimate outputs, such as methane (Bai et al., 2017; Capson-Tojo et al., 2021). In the physicochemical part of ADM1, the model inadequately addresses reactions involving ions and the precipitation processes that occur during AD. Particularly, when considering phosphorus recovery, ion activity, ion pairing and solids precipitation should be described in much more detail (Solon et al., 2017). This requires incorporation of phosphorus, sulfur, and iron in plant-wide modelling. In response to these limitations, many studies have focused on modifying ADM1 to expand its application to more substrates and scenarios.

3. Modifications to the ADM1

To improve model utilization, many modifications to the ADM1 have been proposed. Herein, the extensions are summarized in three aspects, including model structure, kinetics and stoichiometry, and the simplification and adaptation to the ADM1 are also discussed.

3.1. Extension to the model structure

In some cases, key mechanisms are not included in the model (Keroum et al., 2010). This deficiency has led to structural modification of the ADM1. This requires addition of new components (state variables) and processes (reactions), and represents a structural modification to the model. Some modifications are illustrated in Fig. 2.

3.1.1. Extracellular processes and related components

Disintegration and hydrolysis are usually rate limiting steps in the case of a slowly degradable particulate substrate (Ramirez et al., 2009). An accurate description of those processes can improve the predictive ability of the model.

Disintegration describes the conversion of complex solid mixture, X_C, into three biodegradable organic components (X_{pr}, X_{li} and X_{ch}) and inert components (S_i and X_i). In order to simplify the model structure, the original ADM1 assumed that X_C was homogeneous and subject to a single first order disintegration coefficient. In the case when the complex input substrates are not homogeneous, different decomposition efficiencies can be assumed (Mottet et al., 2013). For instance, Yasui et al. (2008) found that degradable organics in the primary sludge contained three distinct kinetically differentiable fractions ($X_{settle\text{-}I}$, $X_{settle\text{-}II}$ and $X_{settle\text{-}III}$) and developed a modified ADM1 structure including separate degradation processes for the three identified solid fractions. The division of X_C into readily and slowly biodegradable solid fractions (X_{CR} and X_{CS}), as shown in Fig. 2a (pathway 1), was proposed based on the different biodegradability obtained from interpreting the methane production curve. The concept was applied to several studies, resulting in reasonable predictions (Garcia-Gen et al., 2015; Jimenez et al., 2014; Montecchio et al., 2019; Mottet et al., 2013). When simulating co-digestion of more than one input substrates, the co-substrates were

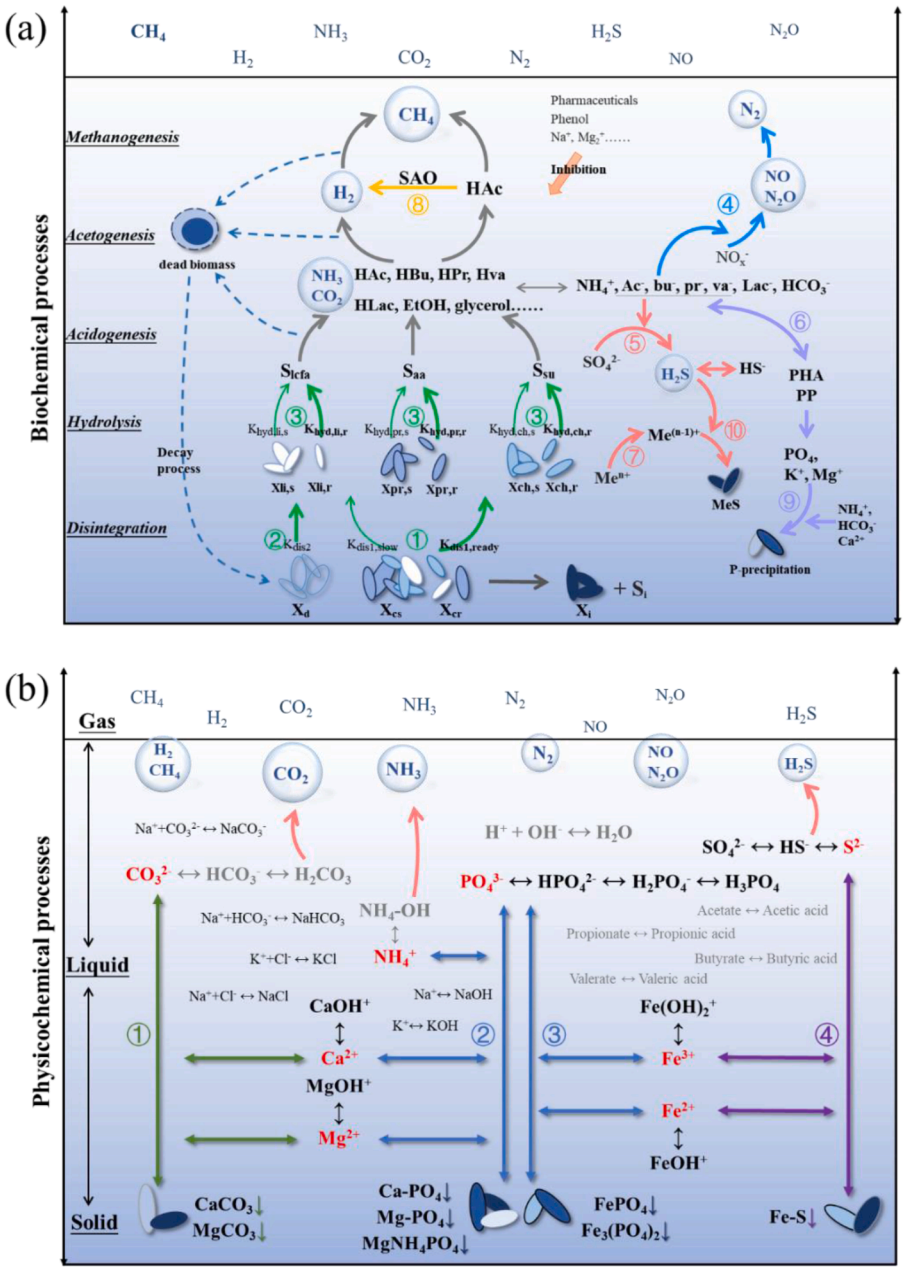

Fig. 2. Conceptual model of biochemical processes (a), including detailed disintegration and hydrolysis processes (green line); nitrate reduction (blue line); conversions of S, Fe and P (red line and purple line) (Batstone et al., 2015); syntrophic acetate oxidation (yellow line) and original processes (black line), and physicochemical processes (b) (Batstone and Flores-Alsina, 2022), including CO_3^{2-} precipitation (dark green line), PO_4^{3-} precipitation (navy blue line) and S^{2-} precipitation (deep purple line), for the modified ADM1.

incorporated by using separate particulate biodegradable components $X_{C\_substrate}$ with different kinetic processes (Donoso-Bravo et al., 2020; Esposito et al., 2011; Zhao et al., 2019). For instance, when simulating the co-digestion of waste activated solid (WAS) and food waste (FW), Montecchio et al. (2019) divided X_C into two terms related to WAS (X_{C_WAS}) and FW (X_{C_FW}). Finally, it is important that only hydrolysis be rate-limiting of solubilization process, and the most common approach is to characterize input solids as a mix of proteins, carbohydrates, lipids, and inerts, and avoid the use of X_C, to both avoid imposing 2nd order hydrolysis kinetics, and allow varying carbohydrate/protein/lipid/inert ratios in the inputs (Batstone et al., 2015; Nopens et al., 2009).

Dead biomass of all species of degrading organisms is recycled to the fraction X_C and undergoes the same disintegration process. However, since disintegration occurs as an initial step of the anaerobic process scheme and decay is continuously performed in a recycling approach throughout the retention time, these two processes are actually not coupled and have different nitrogen contents (Wett et al., 2006). To solve this problem, a modified model ADM1xp was developed, in which the products of the decay process were not completely related to the fraction X_C, but to the X_{pr}, X_{li}, X_{ch} and the new inert fraction (X_p) (Hinken et al., 2014; Wett et al., 2006). X_p represents inert endogenous products, was originally proposed in the ASM1 (Henze et al., 1986), and allows separate tracking of input inerts and endogenous inerts. This modification has widely been accepted (Hagos et al., 2018; Satpathy et al., 2016), and it has been reported by Satpathy et al. (2016) that the ADM1xp could significantly reduce the difference between measured and simulated biogas productions from 48% to 1%. In order to separate the kinetics of biomass decay and degradation of input substrates, a new component, dead biomass (X_d) with different decomposition kinetics, was introduced to the ADM1 to further subdivide the disintegration process (pathway 2 in Fig. 2a) (Garcia-Gen et al., 2013; Montecchio et al., 2019).

Biodegradable disintegration products in the original ADM1 are presented as lumped variables (X_{ch}, X_{pr} and X_{li}), and they are also assumed to be homogeneous, with only one hydrolysis pathway for each of them (Batstone et al., 2002). With the diversification of digestion

substrates, especially when X_C is excluded as an input, the primary particulate substrates may be further fractionated. It was proposed to separate each biodegradable disintegration product into two fractions, i.e., readily biodegradable fractions and slowly biodegradable fractions, and both fractions had different hydrolysis rates (pathway 3 in Fig. 2a) (Bai et al., 2015; Esposito et al., 2011; Garcia-Gen et al., 2015). Bareha et al. (2019) divided the particulate organic matter into protein and non-protein hydrolysable fractions. They were then separately split into four different bioaccessible fractions by a modified "extracellular polymeric substances (EPS)" fractionation method, which was based on successive alkaline extractions ending with strong acid extraction. When simulating the dynamic AD process of lignocellulosic waste, different degradation pathways can be distinguished between cellulose and other biodegradable components. Therefore, the lignocellulosic substrate could be initially disintegrated into three fractions: readily hydrolysable (carbohydrates and proteins), slowly hydrolysable (degradable cellulose) and inert (undegradable cellulose) (Li et al., 2021b; Shi et al., 2014).

3.1.2. Intracellular processes and components

Acidogenesis, acetogenesis and methanogenesis are intracellular biochemical processes. Due to the complexity of these processes, the original ADM1 excludes many intermediate components to maintain a simple structure. Consideration of additional intermediates is a key point in model extension. Some important extensions are introduced as follows and shown in Table 1.

3.1.2.1. Lactate and ethanol. Lactate and ethanol are excluded from the ADM1 due to their low production in most AD systems (Antonopoulou et al., 2012b). However, in the AD systems fed with rapidly degradable carbohydrate-rich substrates or in fermentation processes, lactate and ethanol are important intermediates or by-products (Soda et al., 2011). Lactate (but not ethanol) and other organic acids can accumulate to have a strong effect on pH (Hinken et al., 2014). Therefore, it is desirable to include both lactate and ethanol in the ADM1 under these conditions. An uptake of lactate/ethanol and decay of their degraders were added to the model in terms of four new variables: soluble components (lactate-S_{la}, ethanol-S_{et}) and their degraders (lactate degraders-X_{la}, ethanol degraders-X_{et}). S_{la} and S_{et} are converted from sugar and then decomposed into VFAs and hydrogen with the growth of X_{la} and X_{et} (Soda et al., 2011). This extension has widely been used in AD systems with high carbohydrate substrates, such as organic waste (Soda et al., 2011), silage (Thamsiriroj et al., 2012; Waszkielis et al., 2022), food waste (Parra-Orobio et al., 2020; Satpathy et al., 2016), starch wastewater (Hinken et al., 2014), and sugarcane vinasse (Couto et al., 2022). In contrast, Antonopoulou et al. (2012b) suggested that ethanol was fermented from sugar and would not be further degraded, and X_{et} did not have to be included in the extended model. Garcia-Gen et al. (2014) proposed a new approach presenting the fermentation of components, such as lactate and ethanol, derived from sugar in terms of equivalent glucose fermentation by a generic group of fermenters (X_{fer}) instead of additional microbial groups.

3.1.2.2. Nitrate reduction. Nitrate (NO_3^-) reduction to nitrogen oxides and ultimately to N_2 has significant effects on the electron shift, substrate competition and inhibition during AD, but these processes were not considered in the ADM1. Tugtas et al. (2006) incorporated the NO_3^- reduction processes into the model in order to account for the effects on fermentation and methanogenesis: Butyrate/valerate, propionate, acetate and H_2 were the substrates used by denitrifiers (NO_x degraders-X_{NOx}) in the presence of N-oxides (S_{NOx}) as electron acceptors (pathway 4 in Fig. 2a). Based on this extension, Rousseau et al. (2008) further considered the effects of denitrification on pH in AD systems. Dissimilatory nitrate reduction to ammonia (DNRA) has not been included in the model so far because ammonia production was not observed in sulfide-free and N-oxide-amended cultures, indicating that the primary nitrate reduction pathway is denitrification (Tugtas et al., 2010). DNRA may be considered in the future for more practical purposes.

3.1.2.3. Phosphorus, iron and sulfur transformations. Only carbon (C) and nitrogen (N) transformations were considered in the ADM1, while P, S and Fe transformations were excluded due to limited precedent work at the time of publication and the need to jointly consider these substrates due to their interactions. For sulfate-rich substrates, the sulfate transformations can be described in two different ways (as shown in Table 1). First, soluble sulfate (S_{SO4}) is reduced to sulfide (S_{IS}) by one group of sulfate reducing bacteria (X_{SRB_H2}) using hydrogen as the electron donor (Batstone, 2006). Secondly, a widely used approach has assumed that S_{SO4} is also reduced to sulfides (S_{IS}) with multiple electron donors (S_{bu}, S_{pro}, S_{ac} and S_{h2}) by relevant bacteria species (X_{SRB_c4}, X_{SRB_pro}, X_{SRB_ac} and X_{SRB_H2}) (pathway 5 in Fig. 2a) (Barrera et al., 2015; Fedorovich et al., 2003; Flores-Alsina et al., 2016; Pokorna-Krayzelova et al., 2017). In order to optimize the microaeration process for biogas desulfurization, Pokorna-Krayzelova et al. (2017) extended the ADM1 with one additional process of sulfide oxidation to elemental sulfur by sulfide oxidizing bacteria, X_{SOB}.

P-related components include phosphorus accumulating organisms (X_{PAO}), polyhydroxyalkanoates (X_{PHA}) and polyphosphates (X_{PP}). Their incorporation brings seven new processes: uptakes of S_{va}, S_{bu}, S_{pro} and S_{ac} to form X_{PHA} as well as lysis of X_{PAO}, X_{PP} and X_{PHA} (pathway 6 in Fig. 2a) (Flores-Alsina et al., 2016; Wang et al., 2016). Ferric iron (S_{Fe}^{3+}) is converted to ferrous iron (S_{Fe}^{2+}) by utilizing hydrogen and/or sulfides (S_{IS}) as electron donors (pathway 7 in Fig. 2a) (Flores-Alsina et al., 2016). The extension of P transformations and its close link to the S and Fe cycles are necessary for plant-wide P simulation, especially considering P recovery.

In addition, electron release from zero-valent iron (ZVI) corrosion, H_2 formation from ZVI corrosion and transformation of less biodegradable pollutants (LBPs), were integrated into the ADM1. The modified model could provide more precise strategies for the design, development, and application of ZVI-based anaerobic systems, especially for treating various LBPs-containing wastewaters (Xiao et al., 2013).

3.1.2.4. Syntrophic acetate oxidation. It has been reported that the aceticlastic methanogenesis is likely replaced by a non-aceticlastic methanogenesis, known as syntrophic acetate oxidation (SAO), under high ammonia (NH_4^+) concentrations (Wilson et al., 2012) or high temperature (Wett et al., 2014). To simulate these conditions, a modified ADM1, accounting for the SAO pathway (pathway 8 in Fig. 2a) and SAO bacteria (X_{SAOB}) (Yang et al., 2020), was implemented in AD systems with high temperature or high solid content, which are prone to NH_4^+ inhibition (Montecchio et al., 2017b; Rivera-Salvador et al., 2014; Wett et al., 2014). For instance, Capson-Tojo et al. (2021) modified the model with SAO as acetate-consuming pathway and threshold inhibition function for free ammonia inhibition, and got a better simulation. The correlation coefficient of methane production increased from 0.610 to 0.938.

Some extensions are also proposed under specific conditions. For instance, Fezzani and Cheikh (2009) extended the ADM1 with degradation of phenolic compounds and achieved accurate simulation for the AD of olive mill wastes. Uhlenhut et al. (2018) divided the original uptake of propionate into two more detailed pathways with three new genera of propionate oxidizing bacteria (X_{POB}), and achieved a better fit between simulation and realistic scenarios. The difference between measured and simulated values for mean methane content reduced from 13.4% to 0.6% after that modification.

Table 1
Detailed information of the extensions to the ADM1 model for intercellular processes and components.

	Processes added	Components added	Transformations	Applicable situation/substrate	Refs.
Fermentation	Uptake of lactate; Decay of lactate degraders	lactate - S_{la}; lactate degraders - X_{la}	Sugar $\xrightarrow{X_{su}}$ Lactate Lactate $\xrightarrow{X_{la}}$ Propionate + Acetate	Fermentation process; carbohydrate-rich substrates	Parra-Orobio et al. (2020); Satpathy et al. (2016); Thamsiriroj et al. (2012); Waszkielis et al. (2022)
	Uptake of ethanol; Decay of ethanol degraders	ethanol - S_{et}; ethanol degraders - X_{et}	Sugar $\xrightarrow{X_{su}}$ *Ethanol* *Ethanol* $\xrightarrow{X_{et}}$ Acetate		
Nitrate reduction	Uptake of VFAs with nitrate; Uptake of VFAs with nitrite; Uptake of VFAs with nitric oxide; Uptake of VFAs with nitrous oxide; Uptake of H_2 with nitrate; Uptake of H_2 with nitrite; Uptake of H_2 with nitric oxide; Uptake of H_2 with nitrous oxide; Decay of NO_x degraders	nitrate - S_{NO3}; nitrite - S_{NO2}; nitrogen - S_{N2}; nitric oxide - S_{NO}; nitrous oxide - S_{N2O}; NO_x degraders - X_{NO3}, X_{NO2}, X_{NO}, X_{N2O}	$\text{Nitrate} \xrightarrow[X_{NO3}]{VFAs,\ H_2} \text{Nitrite} \xrightarrow[X_{NO2}]{VFAs,\ H_2} \text{Nitric oxide}$ $\xrightarrow[X_{NO}]{VFAs,\ H_2} \text{Nitrous oxide} \xrightarrow[X_{N2O}]{VFAs,\ H_2} \text{Nitrogen}$	Nitrate-rich wastewater	Tugtas et al. (2006); Rousseau et al. (2008)
Phosphorus, iron and sulfur transformations	Uptake of H_2 with sulfate; Decay of sulfate reducing bacteria	soluble sulfate - S_{SO4}; sulfide - S_{IS}; sulfate reducing bacteria - X_{SRB_H2}	$\text{Soluble sulfate} \xrightarrow[X_{SRB\_H2}]{H_2} \text{Sulfide}$	sulfate-rich substrates	Batstone (2006)
	Uptake of VFAs with sulfate; Uptake of H_2 with sulfate; Decay of sulfate reducing bacteria	soluble sulfate - S_{SO4}; sulfide - S_{IS}; sulfate reducing bacteria - X_{SRB_H2}, X_{SRB_ac}, X_{SRB_pro}, X_{SRB_c4}	$\text{Soluble sulfate} \xrightarrow[X_{SRB\_H2}, X_{SRB\_ac}, X_{SRB\_pro}, X_{SRB\_c4}]{VFA,\ H_2} \text{Sulfide}$		Barrera et al. (2015); Fedorovich et al. (2003); Flores-Alsina et al. (2016); Pokorna-Krayzelova et al. (2017)
	Uptake of H_2S (sulfide oxidation); Decay of sulfide oxidizing bacteria	oxygen - S_{O2}; sulfide oxidizing bacteria - X_{SOB}	$H_2S \xrightarrow[X_{SOB}]{O_2} S$	biogas desulfurization	Pokorna-Krayzelova et al. (2017)
	Storage of VFAs to form polyhydroxyalkanoates; Decay of phosphorus accumulating organisms; Lysis of polyhydroxyalkanoates and polyphosphates	phosphorus accumulating organisms - X_{PAO}; polyhydroxyalkanoates - X_{PHA}; polyphosphates - X_{PP}	VFAs $\xrightarrow{X_{PAO}}$ Polyhydroxyalkanoates Polyhydroxyalkanoates→VFAs	enhanced biological phosphorus removal (EBPR) sludge; plant-wide simulation	Flores-Alsina et al. (2016); Wang et al. (2016)
	Conversion of iron	ferric iron - S_{Fe}^{3+}; ferrous iron - S_{Fe}^{2+}	Ferric iron $\xrightarrow{H_2,\text{sulfides}}$ Ferrous iron	plant-wide simulation	Flores-Alsina et al. (2016)
	Corrosion of ZVI; Degradation of LBPs	zero valent iron – S_{Fe}^{0}; ferrous iron - S_{Fe}^{2+}; less biodegradable pollutants – S_{LBPs}; metabolic products of LBPs – $S_{(CH)}$	$Fe^0 + 2H^+ \rightarrow Fe^{2+} + H_2$ LBPs + H_2→less toxic products	ZVI-based anaerobic systems	Xiao et al. (2013)
Syntrophic acetate oxidation	Syntrophic acetate oxidation; Decay of SAO bacteria	SAO bacteria - X_{SAOB}	Acetate $\xrightarrow{X_{SAOB}}$ $H_2 + CO_2$	Under high ammonia concentration or high temperature	Montecchio et al. (2017b); Rivera-Salvador et al. (2014); Wett et al. (2014)

3.1.3. Physicochemical processes

Physicochemical processes involved in the ADM1 describe the non-biologically mediated processes in AD systems. In the ADM1, only gas-liquid exchange and liquid-liquid (acid-base) reactions were addressed, while ion activity and ion pairing (apart from acid-base pairing) were not included (Batstone et al., 2012). Physicochemical extensions have been extensive since publication of the ADM1 and have been proposed for plant wide (and extra-plant) use via the IWA Physicochemical Model No. 1 (Batstone and Flores-Alsina, 2022) as shown in Fig. 2b. This incorporates much of the extensions discussed below.

Liquid-gas exchange processes for H_2, CH_4 and CO_2 were incorporated in the original ADM1 as two-film (liquid film-controlled) rate expressions. Due to the substrate complexity or changing conditions, it is necessary to consider comprehensive liquid-gas exchanges when new gas components, such as H_2S (Flores-Alsina et al., 2016) and NH_3 (especially above 10 g N/L and under thermophilic conditions) (Zhang et al., 2015), are added to the ADM1. It is noted that gases with high solubility may be gas film controlled (Batstone and Flores-Alsina, 2022). Furthermore, to better describe the acid–base reactions and their effects on the AD processes, more inorganic components and acid/base equilibria should be incorporated into the model. For example, the equilibrium amongst four inorganic phosphorus components (PO_4^{3-}/HPO_4^{2-}/$H_2PO_4^-$/H_3PO_4) was introduced to the model, and a charge balance equation used to calculate the pH value was refined (Zhang et al., 2015). In addition, ion pairing and ion activity have important impacts on physicochemical processes, and have been extended in the ADM1 (Batstone and Flores-Alsina, 2022). Some new components, such as S_{Na}^+, S_K^+, S_{Cl}^-, and ion pairing processes, such as $NaCO_3^- \leftrightarrow Na^+ + CO_3^{2-}$, were considered in the model. Ion strength (as ion activity correction) was corrected by multiplying each ion concentration with an activity coefficient (γ) (Batstone and Flores-Alsina, 2022; Solon et al., 2015). Solon et al. (2015) demonstrated that ion strength correction led to significant differences in predicting the process performance, and activity corrections were more important than ion pairing effects for pH prediction.

Precipitation is the major liquid-solid process, but it was not involved in the original ADM1 due to a wide range of precipitating ions and precipitate types (Ekama et al., 2006). However, liquid-solid reactions are very important in systems with high levels of cations, which can affect both other physicochemical processes and biochemical processes. For instance, struvite ($MgNH_4PO_4$) formation can affect the pH values in AD systems (Britton et al., 2005). In order to improve the model ability to describe the formation rate of precipitates, Zhang et al. (2015) considered calcium ions (Ca^{2+}) and magnesium ions (Mg^{2+}) as two major M^{m+} ions in the model, which could cause 5 major types of precipitates: $CaCO_3$, $MgCO_3$, $MgNH_4PO_4$, $MgHPO_4$, and $Ca_3(PO_4)_2$. Comprehensive P precipitation processes, including the formation of $Ca_3(PO_4)_2$, $Ca_5(PO_4)_3(OH)$, $Ca_8H_2(PO_4)_6$, $MgNH_4PO_4$, $MgHPO_4$, and $KMgPO_4$, were extended to the ADM1 in later studies to simulate P behaviour under the P-rich influent (pathway 9 in Fig. 2a, and pathway 1 and 2 in Fig. 2b) (Flores-Alsina et al., 2016; Wang et al., 2015). Due to strong interactions between S and Fe, Flores-Alsina et al. (2016) and Puyol et al. (2017) extended the precipitation processes required for the P, S and Fe cycles (formation of FeS, and $FePO_4$/$Fe_3(PO_4)_2$, pathway 10 in Fig. 2a, and pathway 3 and 4 in Fig. 2b) by a multiple mineral precipitation model. Subsequently, in order to consider the effects of trace elements on physicochemical processes of AD, the reversible precipation processes involving Fe, Ni, Co, and major anionic components, were added to the model (Maharaj et al., 2018, 2019).

Precipitation kinetics is generally based on the saturation index (SI) that is used to indicate the degree of supersaturation (Kazadi Mbamba et al., 2022). Musvoto et al. (2000) indicated that the precipitation rate only depends on the SI. In order to refine the expression of precipitation kinetics, Kazadi Mbamba et al. (2015) included the effect of precipitate concentration and Lizarralde et al. (2015) considered the delay of nucleation, the influence of crystal seeding and TSS concentration.

Suitable expressions can be introduced into the ADM1 for the extension of precipitation processes. For instance, based on the fundamental relationship in the crystallisation process, the following equation was introduced to describe mechanisms of solids precipitation involving Ca, Mg (Zhang et al., 2015), Fe, Co and Ni (Maharaj et al., 2018):

$$r_{M_{v+}A_{v-}} = k'_{r,M_{v+}A_{v-}} \left[\left([M^{m+}]^{v+} [A^{a-}]^{v-} \right)^{\frac{1}{v}} - k'_{sp,M_{v+}A_{v-}}{}^{\frac{1}{v}} \right]^n \quad (5)$$

where $[M^{m+}]$ and $[A^{a-}]$ denote the concentrations of cations and anions, respectively, $k'_{r,M_{v+}A_{v-}}$ is the precipitation rate constant, $k'_{sp,M_{v+}A_{v-}}$ is the solubility product, v^+ and v^- are the total number of cationic and anionic charges, respectively, and $v = v^+ + v^-$, n is a constant for crystallization of sparingly soluble salts.

3.2. Modifications of kinetics

The kinetics that describe the material conversion mechanism is a fundamental element of the ADM1. Inhibitors present in biochemical processes are incorporated into the model via the use of an inhibition function (I). While the use of Monod functions for microbial growth (or substrate uptake) dominates, variations have been used particularly for hydrolysis, and inhibition, but also biochemical uptake.

3.2.1. Kinetic expressions

In the original ADM1 model, extracellular processes (disintegration and hydrolysis) were assumed to be first-order kinetics, which were independent of microbial activity and proportional to substrate concentration. However, hydrolysis is an enzymatic process where hydrolytic bacteria cover the surface of solids and produce enzymes (Mottet et al., 2013). Vavilin et al. (2008) assessed different hydrolysis models and found that the Contois kinetics provide a better fit at high organic loading rates. The Contois model incorporates a non-parameterized microbial concentration term, and hence describes microbe, as well as substrate limited conditions. Ramirez et al. (2009) developed a modified ADM1 using the Contois kinetics instead of the original first-order kinetics to account for the growth of hydrolytic bacteria. The Contois model was found to be more robust in describing a broad range of experiments with minimal changes to the kinetic coefficients (Mairet et al., 2011). As a result, it has been widely used in simulating high solid content substrates, such as sludge and cattle slurry (Bai et al., 2015; Bareha et al., 2019; Mottet et al., 2013; Normak et al., 2015). In addition, Liotta et al. (2015) proposed a linear function that dynamically express the kinetic constants of three specific processes (disintegration, uptake of acetate and propionate) to account for the effect of the TS content on dry AD.

For intracellular processes, the ADM1 used substrate uptake Monod kinetics to express the biochemical reaction rate (Batstone et al., 2002). The main modification has been the use of growth-based (Siegrist et al., 2002) rather than uptake-based kinetics, and this is mainly perspective, since mathematically, there is no difference as discussed in the ADM1 scientific and technical report. While Monod kinetics have been effective in describing AD processes, alternatives which incorporate maintenance, and hence reduce yield under stress can be applied (and are incompatible with growth-based kinetics) (Kleerebezem and van Loosdrecht, 2008).

3.2.2. Inhibition functions

In the original ADM1, the kinetics of disintegration, hydrolysis, and decay of biomass processes were related only to kinetic constants and substrate concentrations, without taking into account any inhibitors. However, it has been suggested that inhibitors of hydrolysis should be considered due to microbial inactivation and enzyme denaturation under adverse conditions. For example, Normak et al. (2015) introduced hydrolysis kinetics containing VFAs inhibition (I_{TVFA}) to simulate the start-up process of AD of cow manure. Li et al. (2020) considered the

inhibition of hydrolysis caused by high solids content (I_{TS}) and used a non-competitive inhibition function to reflect inhibition of hydrolysis. Furthermore, various inhibitors can increase biomass decay, which is completely neglected in the original ADM1. Sun et al. (2020) developed a low-pH inhibition switching function I_{pH} (Table 2) to describe increased decay at low pH.

For intracellular processes, pH inhibition was implemented using empirical equations, while other inhibitions were presented as non-competitive functions (Batstone et al., 2002). Non-competitive functions have widely been used in literatures, but sometimes they cannot describe inhibition processes accurately. Non-competitive function was only influenced by the concentration of inhibitors and the influence of substrate concentration was ignored. Bai et al. (2017) used the Monod function to simulate the inhibition of free ammonia on VFAs generation during anaerobic fermentation of sludge with high solids content. The determination coefficient of VFAs increased to over 0.95 compared to less than 0.8 when a non-competitive function was used. The Hill function, proposed by Ramirez et al. (2009), has also been used to describe pH inhibition effects (Barrera et al., 2015; Wang et al., 2015). However, these kinetic inhibition functions have limitations, including allowing the reaction to proceed even under unfavourable thermodynamic conditions. Specifically, the uptake of propionate and butyrate is fundamentally impacted by concentration of products (i.e., H_2 and acetate) due to positive Gibbs free energy at elevated concentrations. To address this, the thermodynamic inhibition function (I_{th}, shown in Table 2) of H_2 was introduced into the kinetic expression of the uptake of propionate and butyrate (Shi et al., 2016). This was found to have no impact vs a non-competitive function in biofilm growth kinetics due to interaction, diffusion, and other controlling factors (Batstone et al., 2006b).

Table 2
Inhibition terms added to the ADM1 kinetic expressions.

Inhibition item	Process	Inhibition term	Refs.
I_{TS}	Hydrolysis	$I_{TS} = \frac{1}{1 + S_{TS}/K_{TS}}$	Li et al. (2020)
I_{pH}	Decay of X_{ac}; decay of X_{h2}	specific decay rate $= \frac{b}{IpH}$	Sun et al. (2020)
		$I_{pH} = \begin{cases} exp\left(-3\left(\frac{pHUL - pH}{pHUL - pHLL}\right)^n\right) & if\ pH < pHUL \\ 1\ if\ pH \geq pHUL \end{cases}$	
I_{NH3}	Uptake of acetate	hill function	Ramirez et al. (2009)
		$I_{NH_3} = b\left(1 - \frac{S_{NH_3}^{\alpha}}{KS_{NH_3}^{\alpha} + S_{NH_3,lim}^{\alpha}}\right)$	
	Uptake of acetate	threshold inhibition function	Astals et al. (2018)
I_{VFA}	Uptake of acetate	$I_{TVFA} = \frac{1}{1 + S_{TFVA}/K_{I,TVFA}}$	Boubaker and Ridha (2008); Fezzani and Cheikh (2009)
	Hydrolysis	$I_{VFA} = \frac{1}{1 + \left(\frac{M_{vfa}}{I_{M_{vfa}}}\right)^n}$	Normak et al. (2015)
I_{ac}	Uptake of propionate; uptake of butyrate	$I_{ac} = \frac{1}{1 + S_{ac}/K_{I,ac}}$	Li et al. (2019)
I_{LCFA}	Hydrolysis; Uptake of sugars; Uptake of LCFAs; Uptake of VFAs	$I_{lcfa} = \frac{1}{1 + S_{lcfa}/K_{I,lcfa}}$	Ramirez et al. (2009)
	Uptake of LCFAs; Uptake of acetate; Uptake of H_2	$I_{lcfa} = \frac{1}{1 + S_{lcfa}^2/(K'_{I,lcfa} \cdot X_{I,lcfa})}$	Palatsi et al. (2010)
	Uptake of acetate	Gaussian function $I_{lcfa} =$ $\begin{cases} e^{-2.77259\left(\frac{S_{fa} - K_{I,fa,low}}{K_{I,fa,high} - K_{I,fa,low}}\right)^2} & for\ S_{fa} > K_{I,fa,low} \\ 1\ for\ S_{fa} \leq K_{I,fa,low} \end{cases}$	Arnell et al. (2016); Keucken et al. (2018)
I_{lac}	Uptake of acetate	$I_{lac} = \frac{1}{1 + S_{lac}/K_{I,lac}}$	Thamsiriroj et al. (2012)
I_{Na}^{+}	Uptake of acetate	$I_{Na^+} = \frac{1}{1 + S_{Na^+}/K_{I,Na^+}}$	Hierholtzer and Akunna (2012)
$I_{cations}$	Uptake of acetate	$I_{cations} = \frac{1}{1 + \frac{S_{Na^+}}{K_{I,Na^+}} + \frac{S_{Mg^{2+}}}{K_{I,Mg^{2+}}} + \frac{S_{Ca^{2+}}}{K_{I,Ca^{2+}}} + \frac{S_{K^+}}{K_{I,K^+}}}$	Hierholtzer and Akunna (2014); Song et al. (2018)
I_{Me}^{2+}	All biochemical processes	$I_{Me^{2+}} = \frac{a_1 S_{Me^{2+}} + a_2}{(S_{Me^{2+}})^2 + b_1 S_{Me^{2+}} + b_2}$	Maharaj et al. (2018)
I_{H2S}	Acetogenesis and Methanogenesis	$I_{H_2S} = \frac{1}{1 + S_{H_2S}/K_{I,H_2S}}$	Barrera et al. (2015)
	Acetogenesis and Methanogenesis	$I_{H_2S} = \begin{cases} \left(1 - \frac{S_{H_2S}}{K_{I,H_2S}}\right)^2 & if\ S_{H_2S} < K_{I,H_2S} \\ 10^{-6}\ if\ S_{H_2S} \geq K_{I,H_2S} \end{cases}$	Pokorna-Krayzelova et al. (2017)
I_{PO4}	Uptake of VFAs;Uptake of LCFAs	$I_{PO_4} = \frac{1}{1 + \frac{K_{S,PO_4}}{S_{PO_4}} + \left(\frac{S_{PO_4}}{K_{I,PO_4}}\right)^2}$	Wang et al. (2015)
I_{NOx}	Uptake of acetate; Uptake of H_2	non-competitive inhibition functions	Rousseau et al. (2008); Tugtas et al. (2006)
I_{phenol}	Uptake of acetate	$I_{phenol} = \frac{1}{1 + S_{phenol}^2/K_{I,phenol}}$	Fezzani and Cheikh (2009)
I_{th}	Uptake of VFAs (H_2 inhibition)	$I_{th} = \begin{cases} 1 - \frac{\Delta G_R}{R_{th}T}\ if\ \Delta G_R < 0 \\ 0\ if\ \Delta G_R \geq 0 \end{cases}$	Patón et al. (2017)

In the original ADM1, the effect of acid inhibition was mainly hidden in the empirical pH inhibition function. However, low pH inhibition is partly due to the concentration of free acids, and it is reasonable to include this separately. The non-competitive inhibitory term I_{VFA} was added into the ADM1 to represent the inhibitory effect of high concentration of VFAs on methanogenesis (Boubaker and Ridha, 2008; Fezzani and Cheikh, 2009; Thamsiriroj et al., 2012). Considering the interaction of VFAs, Li et al. (2019) added a non-competitive inhibition function (I_{ac}) to include acetate inhibition on the uptake of propionate and butyrate processes.

The ADM1 includes several commonly used inhibition functions, but specific inhibition functions have been utilized, as summarized in Table 2. Trace elements, such as Fe, Ni and Co, have explicitly been considered by introducing an inhibition term (I^{2+}_{Me}), as they are essential constituents in enzyme systems (Maharaj et al., 2019, 2018). LCFAs inhibition (I_{lcfa}) has also been included in the ADM1, as acetogenesis and methanogenesis are highly sensitive to LCFAs and can be inhibited at high LCFAs concentrations (Beline et al., 2017). Palatsi et al. (2010) proposed a new inhibition function which replaced the K_{Ilcfa} with $K^{'}_{Ilcfa}X_{lcfa}/S_{lcfa}$ (Table 2) to consider a relationship between LCFAs inhibitory substrate concentration and the specific biomass content. In addition, Arnell et al. (2016) used Gaussian function (threshold function that has been used for pH inhibition in ADM1) to describe LCFAs inhibition on the uptake of acetate, which explicitly allowed for determining the onset of the inhibition (Keucken et al., 2018).

Sulfide is also inhibitory to acetogenesis and methanogenesis, and the extension of sulfide inhibition (I_{H2S}) is needed when modelling AD systems with sulfur-rich substrates (e.g. cane-molasses vinasse) to predict the failure of AD (especially methanogenesis) (Barrera et al., 2015). Non-competition inhibition function and a staged inhibition function were used for sulfide inhibitions (Barrera et al., 2015; Pokorna-Krayzelova et al., 2017). Considering the influence of orthophosphate on the biological processes during AD, Wang et al. (2015) modified the ADM1 by including generalized Haldane equations for orthophosphate inhibition (I_{PO4}) into the kinetics for uptake of VFAs and LCFAs. In addition, the ADM1 has also been extended with other inhibition for the acetogenesis and methanogenesis, such as lactate inhibition (Hinken et al., 2014; Thamsiriroj et al., 2012), nitrate inhibition (Rousseau et al., 2008; Tugtas et al., 2006), phenol inhibition (Fezzani and Cheikh, 2009), cation inhibition (Hierholtzer and Akunna, 2012, 2014; Song et al., 2018) and pharmaceuticals inhibition (Fountoulakis et al., 2008).

Expanding the inhibition processes can not only improve model fit, but also help provide strategies to alleviate the inhibition of various adverse factors on AD processes. Acetogenesis and methanogenesis are easily inhibited by intermediates in AD systems, so it is essential to include context specific inhibition in the model to allow realistic simulation of the process.

3.3. Modifications of the model stoichiometry

Stoichiometric coefficients of disintegration ($f_{ch,xc}$, $f_{pr,xc}$, $f_{li,xc}$, $f_{si,xc}$ and $f_{xi,xc}$) represent biodegradable and non-biodegradable fractions of composite solids (X_C). Many researchers have proposed experimental protocols or methodologies for the characterization of substrate composition in relation to ADM1 input variables and have modified the stoichiometric coefficients. Methane production curves obtained from bio-methane potential (BMP) tests have widely been used to estimate biodegradable and inert fractions of the substrates (Baquerizo et al., 2021; Mottet et al., 2013).

Direct physical-chemical analysis was the most basic method to split the complex solids into protein, lipid and carbohydrate (Li et al., 2021c; Ramirez et al., 2009), which include the Lowry's method (Lowry et al., 1951) or Kjeldahl nitrogen for protein content estimation, Soxhlet's method (Luque-Garcia and de Castro, 2004) for lipid content determination, and anthrone reduction method (Dreywood, 1946), Weender analysis (Naumann and Bassler, 1993) or Van Soest method (Van Soest and Wine, 1967) for carbohydrate content measurements. It should be noted that, particularly for high-solids samples, loss or denaturation of organic fractions may occur during analysis. Elemental analysis was proposed by Kleerebezem and Van Loosdrecht (2006) and generalized by Zaher et al. (2009) to convert the elemental composition and COD into ADM1 inputs. Jimenez et al. (2014) proposed a more rapid method by coupling sequential chemical extractions with 3D fluorescence spectroscopy to get the detailed characterization of organic matters. Near infrared spectroscopy is a fast and cost-efficient way to characterize solid wastes content, and it can be used in a partial least square regression model to estimate methane production kinetics (Charnier et al., 2017a, 2017b). Guo et al. (2023) used combined instrumental analyses to achieve a rapid and accurate fractionation of the primary organic matters in the substrates.

The stoichiometry for acidogenesis of sugars can be altered as they may depend on reactor conditions, including redox conditions and pH (Shi et al., 2019). The parameters involved in the original stoichiometry for the acidogenesis ($f_{ac,su}$, $f_{pro,su}$, $f_{bu,su}$, $f_{h2,su}$) are based on the assumption that products are produced in constant proportions, but they may not adequately simulate experimental results (Uhlenhut et al., 2018). In response, Rodríguez et al. (2006) proposed a stoichiometric system with variable acidogenesis products controlled by thermodynamics rather than kinetics. To account for electron-sink capacity (incorporating pH), which highly affects acidogenesis, some other variable stoichiometric systems have been developed and added to the ADM1. These systems depend on the concentration of undissociated acids (Penumathsa et al., 2008), hydrogen partial pressure (p_{H2}) (Thamsiriroj et al., 2012), and NADH/NAD^+ (Shi et al., 2019).

The implementation of the variable stoichiometry system expands the ADM1 applicability to fermentative systems and reduces the parameter numbers to be estimated (Penumathsa et al., 2008; Shi et al., 2019). This development is particularly important due to the fact that the stoichiometric parameters for acidogenesis of sugars are subject to reactor conditions.

3.4. Simplifications/adaptations to the ADM1

In contrast to studies focused on model extension, some research has concentrated on simplifying or adapting ADM1-like models to facilitate their application in processes beyond AD. For instance, in dark fermentation (DF) processes, particularly in some biohydrogen production scenarios, the significance of methanogenesis is diminished or even absent. Therefore, it is prudent to adapt the ADM1 framework to predict the formation of hydrogen and VFAs by excluding the final step of methanogenesis (Gadhamshetty et al., 2010; Pradhan et al., 2016; Valentín-Reyes et al., 2018). In AD or fermentation processes of certain simple substrates, such as sucrose, the initial stage of the process can involve a single substrate instead of X_C, excluding the hydrolysis of protein and lipid (Huang et al., 2018). In addition, a linearized form of ADM1 (LADM) was developed and implemented in a model predictive control (MPC) system to predict the biogas production (Li et al., 2021a).

4. Approaches to calibration and validation of ADM1

4.1. Model calibration

The calibration of the model generally focuses on the kinetic parameters, which would vary with AD conditions and substrates. Kinetic parameters are generally calibrated using the method described in Fig. 3. A large number of kinetic parameters are involved in the model, but only a limited number are contestable (i.e., can be changed in most situations). Those for specific cases can be selected based on previous research, commonly related to the rate-controlling step, which is normally hydrolysis for particulate substrates (Rivera-Salvador et al., 2014) or mathematical algorithms (sensitivity analysis) (Yu et al., 2012). The parameters are estimated by minimizing the error between the

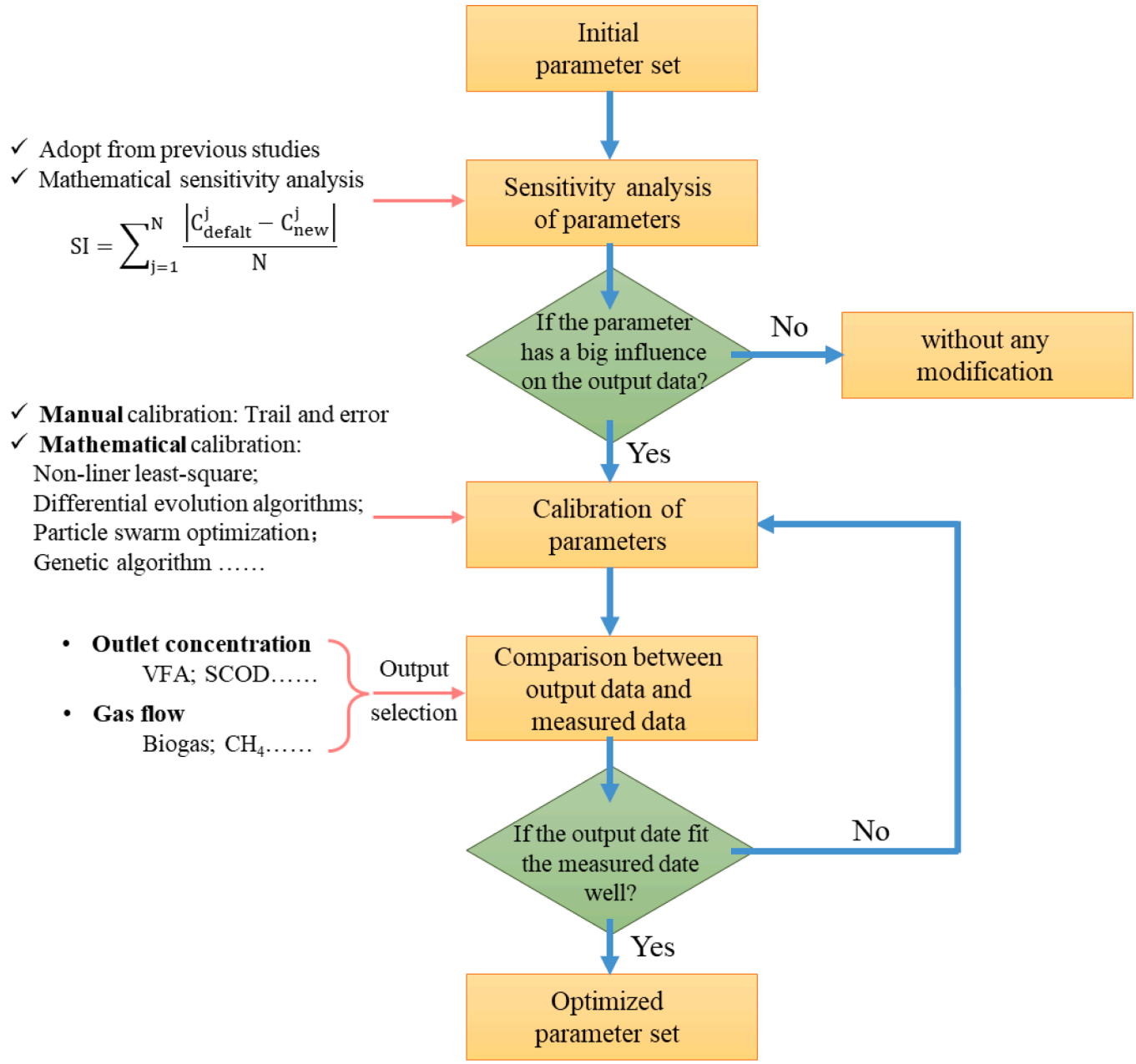

Fig. 3. Modelling methodology used for kinetic parameter calibration.

experimental and simulated data. The "trial and error" method is a simple manual calibration that is suitable for situations where a few parameters need to be calibrated or the simulated results are similar to the experimental data. However, for cases involving many complex parameters, iterative methods (optimization algorithms), e.g., non-liner least-square (Montecchio et al., 2017b), genetic algorithm (Koutrouli et al., 2009), differential evolution algorithms (Rivera-Salvador et al., 2014), implemented simplex method (Hinken et al., 2014), and particle swarm optimization (Bai et al., 2015, 2017), are more efficient and rapid. Any iterative or single step optimisation technique should also include statistical analysis of parameter uncertainty, including joint confidence intervals (Batstone et al., 2009). Experimental methods can also be used to determine kinetic parameters, as demonstrated by Uhlenhut et al. (2018), who used Lineweaver-Burk diagrams to estimate the parameters for uptake of propionate ($k_{m,pro}$ and $K_{s,pro}$). Recently, Ge et al. (2023) used machine learning model to predict the kinetic parameters, and enhanced the performance of ADM1. This indicates machine learning methods can be combined with the traditional mechnism models to improve simulation accuracy.

The description, units, default values, and ranges of reported values of kinetic parameters of the ADM1 are summarized in Table 3. Parameters of hydrolysis and methanogenesis are the most frequently modified parameters. Hydrolysis is considered the rate-limiting step in AD (Feng et al., 2006), and the rate of hydrolysis varies considerably with the substrate. For example, hemicellulose and amorphous cellulose are slower to be hydrolysed than common carbohydrate and protein substrates (Li et al., 2021b). Therefore, the hydrolysis parameters (k_{dis} or k_{hyd}) are more often modified (Table 3). Since methane production is commonly used as a simulation indicator (Montecchio et al., 2019; Ozkan-Yucel and Gökçay, 2010), kinetic parameters for the uptake of acetate and H_2 (k_{m_ac} and K_{s_ac}, k_{m_h2} and K_{s_h2}) which can directly affect methane production, are also frequently modified.

In some specific simulation situations, kinetic parameters of physicochemical processes are also important. For instance, in dry AD of

Table 3
Summary of the reported kinetic parameters in the ADM1.

Symbols	Descriptions	Units	Default values Batstone et al. (2002)	Ranges of reported values	References
k_{dis}	Complex particulate disintegration first order constant	d^{-1}	0.5	0.001–2.2	Biernacki et al. (2013), Boubaker and Ridha (2008), Chen et al. (2016, 2009), Dereli et al. (2010), Ersahin et al. (2007), Fezzani and Cheikh (2009), Gali et al. (2009), Lee et al. (2009), Li et al. (2021c), Montecchio et al. (2017a), Otuzalti and Perendeci (2018), Parra-Orobio et al. (2020), Rivera-Salvador et al. (2014), Satpathy et al. (2016), Shi et al. (2016, 2014), Thamsiriroj and Murphy (2011), Wichern et al. (2009), Yu et al. (2012)
$k_{hyd,ch}$	Carbohydrate hydrolysis first order rate constant	d^{-1}	10	0.1–10	Aichinger et al. (2015), Aldin et al. (2010), Biernacki et al. (2013), Chen et al. (2016, 2009), Derbal et al. (2009), Ersahin et al. (2007), Kerroum et al. (2010), Koch et al. (2010), Li et al. (2021c), Nordlander et al. (2017), Ozkan-Yucel and Gökçay (2010), Parra-Orobio et al. (2020), Rivera-Salvador et al. (2014), Satpathy et al. (2016), Shi et al. (2016, 2014), Uhlenhut et al. (2018)
$k_{hyd,pr}$	Protein hydrolysis first order rate constant	d^{-1}	10	0.0014–10	
$k_{hyd,li}$	Lipid hydrolysis first order rate constant	d^{-1}	10	0.015–10	
$k_{m,su}$	Monod maximum specific monosaccharide uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	30	1.7–37.94	Dereli et al. (2010), Ersahin et al. (2007), Fezzani and Cheikh (2009), Girault et al. (2011), Mendes et al. (2015), Normak et al. (2015), Ozkan-Yucel and Gökçay (2010), Rivera-Salvador et al. (2014)
$K_{s,su}$	Half saturation constant for monosaccharide degradation	$kgCOD \cdot m^{-3}$	0.5	0.12–4.5	
$k_{m,aa}$	Monod maximum specific amino acid uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	50	19.8–50	Aldin et al. (2010), Chen et al. (2016), Dereli et al. (2010), Mendes et al. (2015), Normak et al. (2015), Otuzalti and Perendeci (2018), Rivera-Salvador et al. (2014)
$K_{s,aa}$	Half saturation constant for amino acid degradation	$kgCOD \cdot m^{-3}$	0.3	0.05–0.58	
$k_{m,fa}$	Monod maximum specific long chain fatty acids uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	6	4–24.057	Dereli et al. (2010), Ersahin et al. (2007), Otuzalti and Perendeci (2018), Rivera-Salvador et al. (2014), Wang et al. (2015)
$K_{s,fa}$	Half saturation constant for long chain fatty acids degradation	$kgCOD \cdot m^{-3}$	0.4	0.3–1	
$k_{m,c4}$	Monod maximum specific valerate and butyrate uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	20	5–20.6	Antonopoulou et al. (2012a), Dereli et al. (2010), Ersahin et al. (2007), Kalfas et al. (2006), Koutrouli et al. (2009), Normak et al. (2015), Otuzalti and Perendeci (2018), Ozkan-Yucel and Gökçay (2010), Rivera-Salvador et al. (2014), Thamsiriroj and Murphy (2011), Wang et al. (2015)
$K_{s,c4}$	Half saturation constant for butyrate and valerate degradation	$kgCOD \cdot m^{-3}$	0.2	0.04–0.6	
$k_{m,pro}$	Monod maximum specific propionate uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	13	2.2–18	Barrera et al. (2015), Chen et al. (2009), Ersahin et al. (2007), Girault et al. (2011), Kalfas et al. (2006), Koutrouli et al. (2009), Lee et al. (2009), Normak et al. (2015), Otuzalti and Perendeci (2018), Ozkan-Yucel and Gökçay (2010), Rivera-Salvador et al. (2014), Shi et al. (2016), Sun et al. (2021), Thamsiriroj and Murphy (2011), Wang et al. (2015), Wichern et al. (2009)
$K_{s,pro}$	Half saturation constant for propionate degradation	$kgCOD \cdot m^{-3}$	0.1	0.02–0.6	
$k_{m,ac}$	Monod maximum specific acetate uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	8	4–35	Antonopoulou et al. (2012a), Atallah et al. (2014), Barrera et al. (2015), Boubaker and Ridha (2008), Chen et al. (2016, 2009), Dereli et al. (2010), Ersahin et al. (2007), Fezzani and Cheikh (2009), Girault et al. (2011), Kalfas et al. (2006), Koch et al. (2010), Koutrouli et al. (2009), Lee et al. (2009), Mendes et al. (2015), Montecchio et al. (2017a), Nordlander et al. (2017), Normak et al. (2015), Ozkan-Yucel and Gökçay (2010), Page et al. (2008), Parra-Orobio et al. (2020), Shi et al. (2016, 2014), Sun et al. (2021), Thamsiriroj and Murphy (2011), Wang et al. (2015), Yu et al. (2012), Zhou et al. (2019)
$K_{s,ac}$	Half saturation constant for acetate degradation	$kgCOD \cdot m^{-3}$	0.15	0.05–1.5	
$k_{m,h2}$	Monod maximum specific hydrogen uptake rate	$COD \cdot COD^{-1} \cdot d^{-1}$	35	2–44	Antonopoulou et al. (2012a), Barrera et al. (2015), Chen et al. (2016, 2009), Dereli et al. (2010), Koch et al. (2010), Mendes et al. (2015), Nordlander et al. (2017), Otuzalti and Perendeci (2018), Parra-Orobio et al. (2020), Rivera-Salvador et al. (2014), Shi et al. (2016), Sun et al. (2021), Thamsiriroj and Murphy (2011), Wichern et al. (2009), Zhou et al. (2019)
$K_{s,h2}$	Half saturation constant for uptake of hydrogen	$kgCOD \cdot m^{-3}$	7×10^{-6}	1×10^{-6}–2.5×10^{-4}	
k_{dec}	Decay rate for organisms	d^{-1}	0.02	0.02	/
$K_{I,h2,c4}$	Hydrogen inhibitory concentration for C_4 degrading organisms	$kgCOD \cdot m^{-3}$	1×10^{-5}	5×10^{-8}–1×10^{-5}	Koch et al. (2010), Wichern et al. (2009)
$K_{I,h2,fa}$	Hydrogen inhibitory concentration for FA degrading organisms	$kgCOD \cdot m^{-3}$	5×10^{-6}	5×10^{-6}	/
$K_{I,h2,pro}$	Inhibitory hydrogen concentration for propionate degrading organisms	$kgCOD \cdot m^{-3}$	3.5×10^{-6}	4.6×10^{-8}–3.5×10^{-6}	Koch et al. (2010), Wichern et al. (2009)
$K_{I,NH3,ac}$	Inhibitory free ammonia concentration for acetate degrading organisms	$kgmole \cdot m^{-3}$	0.0018	0.0018–0.0223	Boubaker and Ridha (2008), Fezzani and Cheikh (2009), Normak et al. (2015), Wichern et al. (2009)
$pH_{LL,ac}$	pH level at which there is full inhibition of acetate degradation	–	6	6	/
$pH_{UL,ac}$	pH level at which there is no inhibition of acetate degrading organisms	–	7	7	/

(*continued on next page*)

Table 3 (*continued*)

Symbols	Descriptions	Units	Default values Batstone et al. (2002)	Ranges of reported values	References
$pH_{LL,h2}$	pH level at which there is full inhibition of hydrogen degrading organisms	–	5	5	/
$pH_{UL,h2}$	pH level at which there is no inhibition of hydrogen degrading organisms	–	6	6	/
$pH_{LL,acid}$	pH level at which there is full inhibition	–	4	4–6	Wichern et al. (2009)
$pH_{UL,acid}$	pH level at which there is no inhibition	–	5.5	5.5–8.5	Wichern et al. (2009)

cardboard, in addition to the decrease in the first-order hydrolysis rate (k_{hyd_ch}), a reduced gas transfer resulted in a significant decrease in the liquid/gas mass transfer coefficient, k_T, from its default value of 200 d^{-1} for wet AD of activated sludge to 0.5 d^{-1} (Abbassi-Guendouz et al., 2012). Apart from kinetic coefficients (gas transfer, solids precipitation), most parameters in the physicochemical model are fundamentally fixed by free energy, and are not contestable.

4.2. Model validation

The validation of the model is to fit the outputs of the model with the experimental results, which is also the evaluation of the model. The goodness of outputs of simulation can be evaluated by means of the Nash Sutcliffe Efficiency Coefficient (NE), the Root Mean Square Error (RMSE) (Jimenez et al., 2014), the Correlation Coefficient (CC) (Montecchio et al., 2019), Theil's inequality coefficient (TIC) (Wang et al., 2015), regression or correlation coefficient (R^2) (Jimenez et al., 2014; Mottet et al., 2013), mean relative absolute error (MRAE) or mean absolute error (MAE) (Barrera et al., 2015; Li et al., 2020) et al. Finally, parameter uncertainty (confidence interval) can be used to determine model validity as expressed through parameters (a narrow region identifies a high confidence in model parameter) (Batstone et al., 2009).

The model can be used as a validation platform to verify the experimental results and explain the process mechanism by model parameters, structures and simulation results (Fig. 4). Feng et al. (2006) identified that hydrolysis was not a rate-limiting step in the AD of blackwater since the output of ADM1 was not sensitive to the distribution ratio amongst carbohydrates, proteins and lipids. Li et al. (2021c) explained the inhibitory effect of lignin on the AD process by comparing the hydrolysis kinetic parameters of the expanded component (cellulose). The model results can also be combined with microbial analysis to verify and explain microbial activity that is difficult to observe with macroscopic experimental phenomena. For instance, Montecchio et al. (2017b) validated the microbiological activity of SAO with the extended ADM1, and the simulation results showed the variation of microorganisms involved in the SAO pathway. Yang et al. (2020) used the ADM1 to simulate the bioaugmentation to alleviate ammonia inhibition during AD and analyse effects of different bioaugmentation strategies on the methanogenic process.

5. Practical applications of the ADM1

The ADM1 was developed as a generalized model, but focused on sewage sludge (Batstone and Keller, 2003; Batstone et al., 2004). With the modification of the model, the model can be more widely used in different AD systems with complex substrates, such as food waste, agriculture waste or other co-substrates with sewage sludge. So far, the modified ADM1 has been used to simulate the lab-scale or full-scale AD processes in reactors including continuously stirred tank reactor (CSTR), upflow anaerobic sludge bed reactor (UASB), anaerobic baffled reactors (ARB), two-phase anaerobic digestion, temperature-phase anaerobic digestion, anaerobic membrane bioreactor (AnMBR), and good

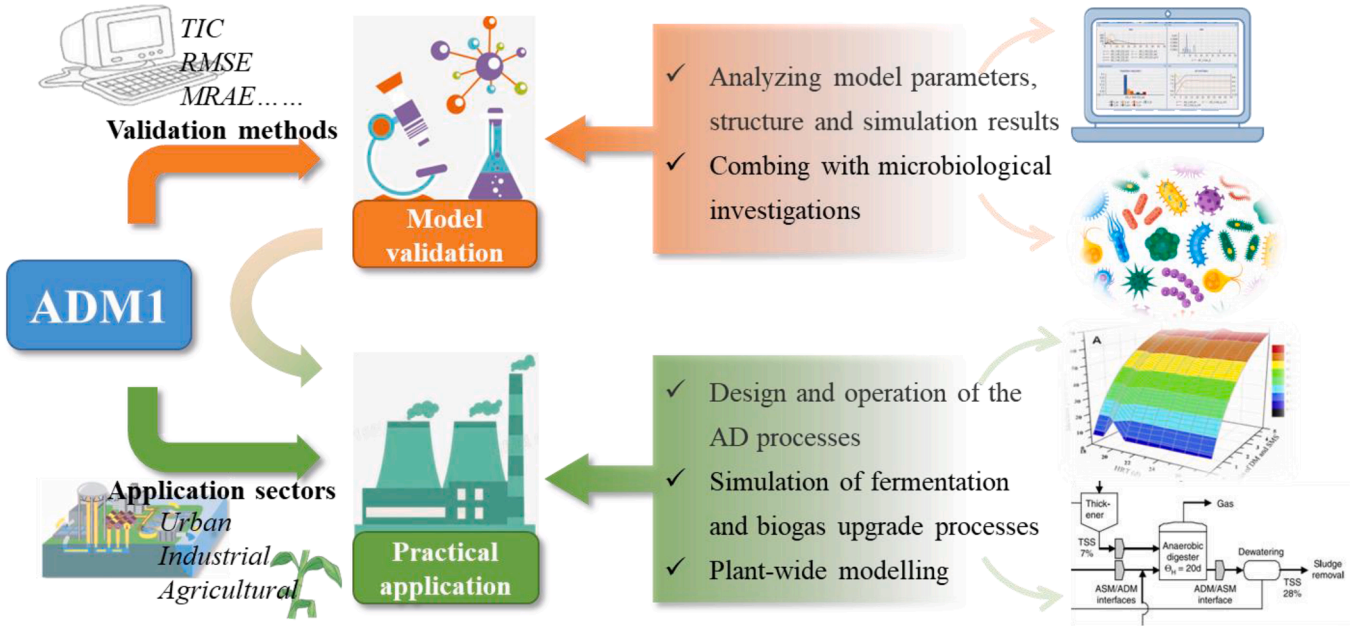

Fig. 4. Validation and application of the ADM1.

simulation results on various output indexes were obtained, as shown in Table 4.

The well-fitted ADM1 model can be applied to simulate AD processes of urban, agricultural and industrial wastes as presented in Table 4. For urban application, the ADM1 has been used for simulation and design of AD systems of urban organic wastes, such as food and garden wastes (Curry and Pillay, 2012; Fitamo et al., 2016), municipal wastewater (Ozgun, 2019), grey water, black water, faeces (Elmitwalli et al., 2006, 2011), and primary or waste activated sludges from water resource recovery facilities (WRRFs) (Baquerizo et al., 2021). The ADM1 is also useful in agricultural applications, such as AD processes of grass silage (Koch et al., 2010; Wichern et al., 2009), sweet sorghum extract (Antonopoulou et al., 2012a), and manure (Li et al., 2020; Page et al., 2008). The industrial applications of the ADM1 are much more extensive (as shown in Table 4) and more complex substrates are involved, such as various kinds of industrial wastewater (Ersahin et al., 2007; Hinken et al., 2014), olive mill solid waste (Boubaker and Ridha, 2008), and vinasse from sugarcane ethanol distillation (Barrera et al., 2015; Couto et al., 2022).

The ADM1 can be used as a management tool for the design and operation of the engineered AD processes in practice (Fig. 4). The AD start-up process is one of the most important issues when a new biogas plant is built or restarted (Normak et al., 2015). This can be unstable or fail due to poor inoculum (Pandey et al., 2010, 2011) or high organic loading rate (OLR) (Zhao et al., 2010). The extended ADM1 can help better predict the start-up process, such as the activity of microorganisms (Jablonski and Lukaszewicz, 2014; Zhao et al., 2010) and dynamic changes of VFAs (Shi et al., 2016), and to provide a start-up procedure, including dynamic control (Batstone et al., 2010). Normak et al. (2015) simulated the uninoculated start-up of the anaerobic digestion of cattle slurry using the modified ADM1 with an inhibition phase, and identified an inhibitory threshold value of VFAs to hydrolysis of 9.87 $g{\cdot}L^{-1}$ during the start-up period. During stable operation, the model can be used to adjust AD condition and realize the maximum recovery of energy and other by-products with the minimum manual effort or ancillary measurements. OLR and hydraulic retention time (HRT) are significant operational parameters in the AD process. Based on simulation using a modified model, Mendes et al. (2015) concluded that the optimum HRT of the mesophilic anaerobic sludge digestion system was in the range of 6–9 days, and organic shock loading rate above 35 $kg{\cdot}m^{-3}{\cdot}d^{-1}$ would negatively impact performance of the reactor or cause it to fail. This application was supported by Montecchio et al. (2017a), who proposed that the maximization of the methane and energy production for one unit of digester volume in thermophilic biogas plants fed with waste activated sludge was achieved at HRTs range of 10–12 days. Some researchers used the ADM1 to predict the collapse threshold of the anaerobic digester (Boubaker and Ridha, 2008; Koutrouli et al., 2009). When multiple substrates are co-digested, the model can be used to determine the optimal ratio between different substrates to maximize the biogas production (Sanaye et al., 2022; Zaher et al., 2009; Fitamo et al., 2016). For instance, Zhou et al. (2019) simulated the anaerobic co-digestion (AcoD) of WAS and maize with different mixing ratios, and demonstrated the optimal ratio was 2: 1. Zhou et al. (2020) developed a rule-based proportional-integral-derivative (PID) controller for the feeding control of the AcoD process, which were combined with the ADM1 to keep methane production stable at the setpoint, resisting the disturbances and maximizing methane production.

The development of plant-wide modelling is driven by the fact that the sludge originates from the wastewater treatment and that the nature of the sludge is closely related to the wastewater treatment process. In addition, return streams from digestion are a significant load on the main treatment process (Monje et al., 2022). In order to compare the performance of different control strategies in a unified framework, the Benchmark Simulation Model No. 2 (BSM2) was presented as a plant-wide model, which contains both ASM series and the ADM1 (Gernaey et al., 2014, 2006; Vreck et al., 2006). With the emphasis on P recovery, in order to simulate the P recovery in wastewater treatment processes, Batstone et al. (2015) and Flores-Alsina et al. (2016) proposed a plant-wide phosphorus model (including S and Fe) based on BSM2. Plant-wide modelling of wastewater treatment has been a key focus, particularly in the development of commercial software (Batstone et al., 2015).

The application scope of the modified ADM1 has significantly been expanded. Beyond its conventional use in the AD process, the modified models can offer valuable insights into process optimization, substrate utilization, and product formation of the fermentation processes. Various kinds of valuable by-products can be produced during the anaerobic fermentation, such as lactate, VFAs and H_2, and the modified ADM1 can be used to predict the production of those compounds and regulate optimal fermentation conditions (Guellout et al., 2018; Shi et al., 2016).

In addition, biogas upgrading processes are crucial for enhancing the quality and potential utilization of biogas. The ADM1 has been extended and adapted to facilitate the simulation of biogas upgrading by biogas desulfurization. In a study of Oliveros-Muñoz et al. (2021), the modified ADM1-S/O was used to optimize microaeration conditions, revealing that the optimal initiation time for microaeration was day 11, whereas the dissolved oxygen concentration in the digester was 1.936×10^{-4} ppm. However, the ADM1 application in biogas upgrading processes remains relatively limited. In the future, the model could potentially serve as a useful tool for exploring additional biogas upgrading processes, such as CO_2 removal and CH_4 enrichment.

In summary, the ADM1 has been proved to be helpful in the full-scale biogas plants to simulate the organic waste treatment processes (Donoso-Bravo et al., 2020) and to provide useful strategies for plant designers and practitioners by predicting possible problems and formulating effective mitigation schemes.

6. Future research directions, perspectives and challenges

The ADM1 still has some limitations. Firstly, although previous modifications of the model have broadened its scope, as shown in Table 4, there are still some unsatisfactory or even neglected areas. For example, during the co-digestion of WAS with beverage wastewater, although the biogas production was predicted well, the VFAs and total ammonia nitrogen (TAN) underperformed (Donoso-Bravo et al., 2020), and few studies have simulated the change of amino acids, sugars and LCFAs. In many cases, this is because the underlying mechanisms have not been fully investigated. Secondly, high VFAs or ammonia can inhibit hydrolysis (Chen et al., 2016), but there is very little literature describing this in an ADM1 context. Finally, as summarized in Table 4, most ADM1 simulations of other substrates (such as food waste and agricultural waste) besides sludge are still at the lab-scale level, and verification of the model in full-scale plants is lacking. Additionally, in order to improve biogas production, these substrates have been co-digested with sludge, causing changes in feed properties. However, model simulation studies on the co-digestion have also been performed in the lab-scale.

To address the abovementioned limitations and promote the application of the ADM1, it is necessary to consider complete processes in the models. A more comprehensive consideration of the intermediate production and uptake processes is needed to improve the poor fitting of the current model to the intermediate products. Additionally, the inhibition functions of hydrolysis need further development to make the model work in both normal and extreme AD conditions. As the model is extended, the number of parameters involved is gradually increasing, which requires a fast and accurate methodology for parameter estimation and calibration. Moreover, some novel biogas upgrading processes, such as CO_2 removal and CH_4 enrichment, are still promising applications of the modified ADM1 in future research. In addition to biogas, the ADM1 can be further modified and aid in understanding and optimizing the production of valuable intermediates such as ethanol, lactic acid,

Table 4
Application of the ADM1 to different anaerobic digestion scenarios.

	Substrates	Conditions	Scale and Reactor	Simulation items	Simulation results and analysis	Refs.
Urban applications	PS+WAS	Part of a WTTP Mesophilic	Full-scale CSTR	Biogas, CH_4% TS, VS	The differences between the ADM1 results are all within 2%	Shang et al. (2005)
	Sewage, grey water, black water and faeces	Part of urban sanitation Low and high temperature (15 - 35 °C)	Full-scale; UASB + UASB septic-tank	CH_4 flow, CH_4% COD, COD removal	Determination of a suitable design for each system	Elmitwalli et al. (2006)
	OFMSW + WAS	Mesophilic	Full-scale	Biogas flow, CH_4%, CO_2% pH, COD, TVFA, IN, IC	Acceptable simulating results	Derbal et al. (2009)
	Domestic wastewater	Mesophilic	Pilot-scale UASB	Biogas flow pH, TCOD, SCOD	With average experimental values within 10% of the simulated results	Lohani et al. (2016)
	Municipal wastewater	Mesophilic	Full-scale	CH_4 flow COD, alkalinity, pH	Acceptable simulating results	Ozgun (2019)
	Urban wastewater	Part of a WRRF Mesophilic	Full-scale	Biogas flow, CH_4% COD, TSS, VSS, N, P	Acceptable simulating results	Baquerizo et al. (2021)
	Food waste	Continuous mode Mesophilic	Pilot-scale Two-stage (CSTR+ ADR)	Biogas flow, VFAs, pH	In CSTR: R^2 (pH)>0.85, R^2(biogas) =0.42 In ADR: R^2 (pH)=0.81, R^2(biogas)=0.96, R^2 (VFAs)=0.97	Yu et al. (2012)
		Semi-continuous mode Thermophilic	Lab-scale	CH_4 flow pH, TCOD, acetate, NH_4^+	Average absolute percent relative error based on methane optimization: 13.7% of CH_4, 9.4% of pH, 58.2% of NH_4^+, 110.2% of ammonia, 70.16% of TCOD	Atallah et al. (2014)
	Fruit and vegetable wastes	Semi-continuous mode Mesophilic	Lab-scale CSTR	Biogas flow pH, VS	Acceptable simulating results	Garcia-Gen et al. (2015)
	Food and garden waste	Thermophilic	Lab-scale CSTR	CH_4 flow NH_4^+, VFAs	Simulate the optimal feedstock composition for CH_4 production	Fitamo et al. (2016)
	Food waste +WAS	Semi-continuous mode Mesophilic	Lab-scale CSTR	CH_4 flow pH, TAN, COD	Nash Sutcliffe Efficiency Coefficient=0.76–0.82 Correlation Coefficient=0.9–0.96 Root Mean Squared Error=0.09–0.12	Montecchio et al. (2019)
Industrial applications	Corn processing wastewaters	Mesophilic	Full-scale EGSBR	CH_4 flow pH, COD	The mean absolute relative error values are 18%, 10%, and 1%, respectively for methane production, COD and pH	Ersahin et al. (2007)
	Olive mill wastewater and solid waste	Semi-continuous mode Mesophilic	Lab-scale Tubular digesters	Gas flow, CH4%, CO2% pH, TVFA	Acceptable simulating results; the reactor failure at high OLR and short HRT was predicted by model	Boubaker and Ridha (2008)
	Evaporator condensate from pulp mill	Semi-continuous mode Mesophilic	Lab-scale 5 L glass contact CSTR	CH_4 flow, CH4% SCOD, COD removal, pH, VFA	Acceptable simulating results	Silva et al. (2009)
	Opium alkaloid effluents	Continuous mode Mesophilic	Lab-scale UASB	CH_4 and CO_2 flow pH, COD	Acceptable simulating results except biogas flows in the latter periods	Dereli et al. (2010)
	Starch wastewater	Continuous mode Mesophilic	Lab-scale UASB	CH_4 flow Lactate, VFAs, COD	Acceptable simulating results	Hinken et al. (2014)
	Vinasse	Mesophilic	Lab-scale 3.5 L UASB reactor	Biogas and H_2S flow COD, pH, SO_4^{2-}, VFAs	Acceptable predictions; predict failure of AD when the sulfate loading rate increased	Barrera et al. (2015)
		Part of biogas plant Mesophilic	Full-scale covered in-ground anaerobic reactor	Biogas flow, H_2S %, CH_4%	The values of relative absolute error are under 20%	Silva Neto et al. (2019)
		Continuous mode Thermophilic	Lab-scale	H_2 flow Lactate, VFAs	The stability of the Markov Chain was greater than 96%; modelling combined with microbial analysis	Couto et al. (2022)
	Confectionery effluents	Mesophilic	Full-scale EGSBR	CH_4 flow COD, TVFA, pH	MRAE for COD, CH_4 flow, TVFA and pH were 22%, 16%, 29% and 1%	Dereli (2019)
	Industrial wastewater	Mesophilic	Lab-scale AnMBR	CH_4 flow Inhibitions by free ammonia and cations	Long SRT values cause high CH_4 rate for MBR; inhibitions of free ammonia and cations to osmosis membrane	Song et al. (2018)

(*continued on next page*)

Table 4 (*continued*)

	Substrates	Conditions	Scale and Reactor	Simulation items	Simulation results and analysis	Refs.
		Mesophilic	Full-scale Internal circulation reactor	CH_4, CO_2 and H_2S flow pH, TVFA, COD, SO_4^{2-}, IN (NH_x), IP ($H_xPO_4^{3-x}$)	Average deviations <15%	Feldman et al. (2018)
Agricultural applications	Sweet sorghum extract	Batch mode Mesophilic	Lab-scale 1350 mL flasks	H_2, flow pH, VFAs	Acceptable simulating results except overestimated pH	Antonopoulou et al. (2012b)
		Continuous Mesophilic	Pilot-scale Two-stage CSTR	CH_4 and biogas flow pH	The deviation values for CH_4: 1.9% (15d HRT) and 1.1% (10d HRT); the deviation of pH and CH_4%<5%	Antonopoulou et al. (2012a)
	Grass silage	Semi-continuous mode Mesophilic	Lab-scale 35 L fermenters	Gas flow and composition, H_2 pH, TS, VFAs	Final square error sum=28.3	Wichern et al. (2009)
		Mesophilic	Lab-scale Two-loop reactor	Biogas flow, CH_4%, CO_2%, TN, NH_4^+, VFAs	Acceptable simulating results (75% coverage) except CH_4% and CO_2%	Koch et al. (2010)
	Vegetable crop residues	Batch mode Mesophilic	Lab-scale 500 ml flasks	CH_4	R^2 (CH_4) =0.982	Li et al. (2021c)
	Dairy manure	Semi-continuous mode Mesophilic	Lab-scale bench-scale digester	Biogas flow, CH_4%, CO_2% COD reduction, NH_4^+, VFAs	CH_4%, CO_2%, TVFA and COD reduction fit well; Biogas and NH_4^+ were overpredicted	Page et al. (2008)
		Mesophilic	Full-scale plug-flow digesters	Biogas flow, CH_4%, CO_2% COD reduction, NH_4^+, VFAs	Biogas, biogas composition and COD fit well; VFAs and NH_4^+ were overpredicted	
	Pig manure	Semi-continuous mode Mesophilic	Lab-scale	CH_4 flow SCOD, NH_4^+, PO_4^{3-}	R^2(methane)=0.92; R^2(SCOD)=0.852; R^2(NH_4^+-N) =0.728; R^2(PO_4^{3-}) =0.685	Li et al. (2020)
	Dairy manure + Mushroom substrate	Semi-continuous mode Mesophilic	Lab-scale CSTR	CH_4 flow pH	Acceptable simulating results	Shi et al. (2014)

PS: primary sludge;.
OFMSW: organic fraction of municipal solid waste;.
TPAD: temperature-phased anaerobic digestion;.
EGSBR: Expanded granular sludge bed reactor;.
ADR: advective-diffusive reactor.

and VFAs. In addition, chain elongation is a potential process for the production of valuable biochemicals and biofuels, such as caproate and caprylate, from organic wastes. However, the ADM1 model has not been applied in this area. Because of the open structure and common nomenclature of the ADM1, the model may be valuable in other fields as well.

In the long term, with the development of modern instrumental analytical technology, especially the molecular biological technology, a deeper understanding of the mechanism of the anaerobic fermentation and digestion processes will be achieved. It is necessary to continuously improve the ADM1 based on this deeper understanding, so that it can more accurately simulate these anaerobic processes.

7. Conclusions

The ADM1 serves as a robust and versatile tool for evaluating the performance of anaerobic treatment processes. This review aims to enhance the current understanding of the ADM1 and establish a solid foundation for future model development. The main conclusions derived from this review can be summarized as follows:

(1) The key elements of the ADM1, including components, processes, stoichiometric coefficients, kinetic expressions and the relevant parameters, have undergone modifications to serve varying purposes since the original model was proposed.
(2) Modifications to the model structure have predominantly focused on extending its scope to include components and processes that were absent in the original model. Notable modifications include the incorporation of uptake of lactate and ethanol, nitrate reduction, phosphorus-iron-sulfur transformation and SAO. Furthermore, the IWA Physicochemical Model has been proposed to encompass physicochemical processes, incorporating such factors as ion activity, ion pairing and precipitation.
(3) Microbial effects on hydrolysis have been accounted for by replacing first-order kinetics with Contois kinetics. However, a more comprehensive exploration of high VFA or ammonia inhibitions on hydrolysis is needed in the future.
(4) Variable stoichiometric systems, tailored to redox conditions and pH, offer improved accuracy in describing acidogenesis of sugars compared to using constant stoichiometric coefficients.
(5) The parameters have been estimated to minimize errors between the experimental data and model predictions by either “trial and error” approach or dedicated optimization algorithms. The parameters related to hydrolysis and methanogenesis have been most frequently adjusted to enhance the accuracy of AD process simulations.
(6) The ADM1 has a versatile range of urban, agricultural and industrial applications. In addition to AD processes, the modified model can also be used for fermentation and biogas upgrading processes. However, there is still a lack of full-scale model applications to substrates other than sewage sludge.
(7) It is highlighted that the ADM1 can be further developed based on the in-depth understanding of the anaerobic treatment processes of organic wastes and the need to recover of valuable products.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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