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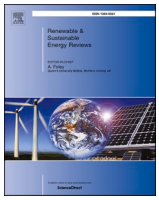

Amendments to model frameworks to optimize the anaerobic digestion and support the green transition

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ABSTRACT

The current world energy system is still heavily dependent on fossil resources (non-renewable and depletable). Anaerobic digestion (AD) has been pointed out as a great strategy for waste and wastewater management while producing biogas that can be upgraded to biomethane. Mathematical models can provide insights into understanding and analyzing important aspects of any process, while minimizing experimental effort, risk, and cost. However, modeling as means to predict, control, and optimize the performance of biological processes on pilot or higher scale is rather scarce. The so-called "BioModel" and Anaerobic Digestion Model No. 1 (ADM1) are well-known model frameworks to understand, characterize, and simulate the anaerobic digestion (AD) processes. Multiple amendments, modifications, and additions occurred during the past years in both frameworks. Therefore. the present article aims to review the most relevant updates made to these models and enlighten the perspectives on the role of kinetic modeling in bio-based gas production. The potential of the existing highly efficient AD models to serve as a basis to develop, predict, and finally support the biogas and bio-methanation processes at a higher scale is discussed.

1. Introduction

The IPCC has recently disseminated the urgent need for a decrease in the worldwide temperature by 1.5 °C to alleviate the current and future generations from the adverse impacts on ecosystems [1]. To achieve this goal, it is pivotal that the industries will adopt and implement net-zero emissions strategies as soon as possible and no later than 2050. For example, the European Union (EU) aims to reduce GHG emissions by 55% by 2030 and establish Europe as climate-neutral by 2050 [2]. While it is anticipated that new technologies will be needed in the long term to establish carbon neutrality, the existing solutions will contribute to fulfilling the short-term targets.

For instance, the gas sector is planned to act as a bridge toward the new green era and considering the current market and geo-political situation, the importance of natural gas as an energy carrier is recently highlighted for securing the domestic and affordable energy supply [3]. To promote the sustainable gas production and consumption, Denmark as a pioneer country – as of June 2023, the amount of biogas produced through AD and integrated into the natural gas grid has surpassed 39% [4] –targets to have 100% green gas on the grid by 2030 to avoid energy insecurities in the future [5].

The growth of global biofuel production is highly driven by policies encouraging energy security and the reduction of carbon emissions. Despite increasing attention to the biofuel sector, biogenic emissions are in parallel increased. To open the road for a sustainable utilization of biofuels, CO_2 credits, and taxation are key parameters for greenifying the gas sector. In the long run, similar incentives can boost the greenification of intensively carbon-emitting industries (e.g. cement, lime, and steel industries). Released carbon has to be better utilized and biomethanation can be a game-changer herein. Biomethanation can be either applied after AD to couple the biogenic CO_2 with H_2 or upgrade syngas/pyrolysis gases that are enriched in $CO{:}CO_2{:}H_2$ or in general, being exploited in CO_2 emitting industries [6,7]. Nowadays, more than 1000 biomethanation plants are operating in the EU and the overall number is following an increasing trend. While the industrial sector is already producing more than 32 TWh of green gas by 2021, it is aimed that it could substantially enlarge the production to 370 TWh by 2030 and reach 1170 TWh by 2050 [8]. Hence, there is huge potential for expanding the biomethanation process.

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Nomenclature

Abbreviations

AD	Anaerobic Digestion
ADM1	Anaerobic Digestion Model No. 1
AGR – IC	Anaerobic Granular Reactor – Internal Recirculation
COD	Chemical Oxygen Demand
CSTR	Continuously Stirred Tank Reactor
EU	European Union
FAN	Free Ammonia Nitrogen
FBA	Flux Balance Analysis
GHG	Greenhouse Gas
HRT	Hydraulic Retention Time
IPCC	Intergovernmental Panel on Climate Change
ODE	Ordinary differential equation
PABR	Periodic Anaerobic Baffled Reactor
RMSE	Root Mean Square Error
SAO	Syntrophic Acetate Oxidizers
STR	Solid Retention Time
TWh	Terawatt hour
UASB:	Upflow Anaerobic Sludge Blanket Reactor
UASB–AF,	Upflow Anaerobic Sludge Blanket – Anaerobic Filter
VFA	Volatile Fatty Acids
VS	Volatile Solids

Notations

C	Carbon
CO_2	Carbon Dioxide
CH_4	Methane
HCO_3^-:	Bicarbonate
$H_xPO_4^{3-x}$:	Phosphate
H_xS^{2-x}:	Sulphite
H_2	Hydrogen
H_2S	Hydrogen Sulphide
K^+	Potassium
$K_{I,NH3}$	Ammonia Inhibition Parameter
N	Nitrogen
Na^+	Sodium
$P_{organic,P}$	Organic phosphorus
S	Sulphur
S_{H^+}	Hydrogen Ion
SO_x^{2-}	Sulfate

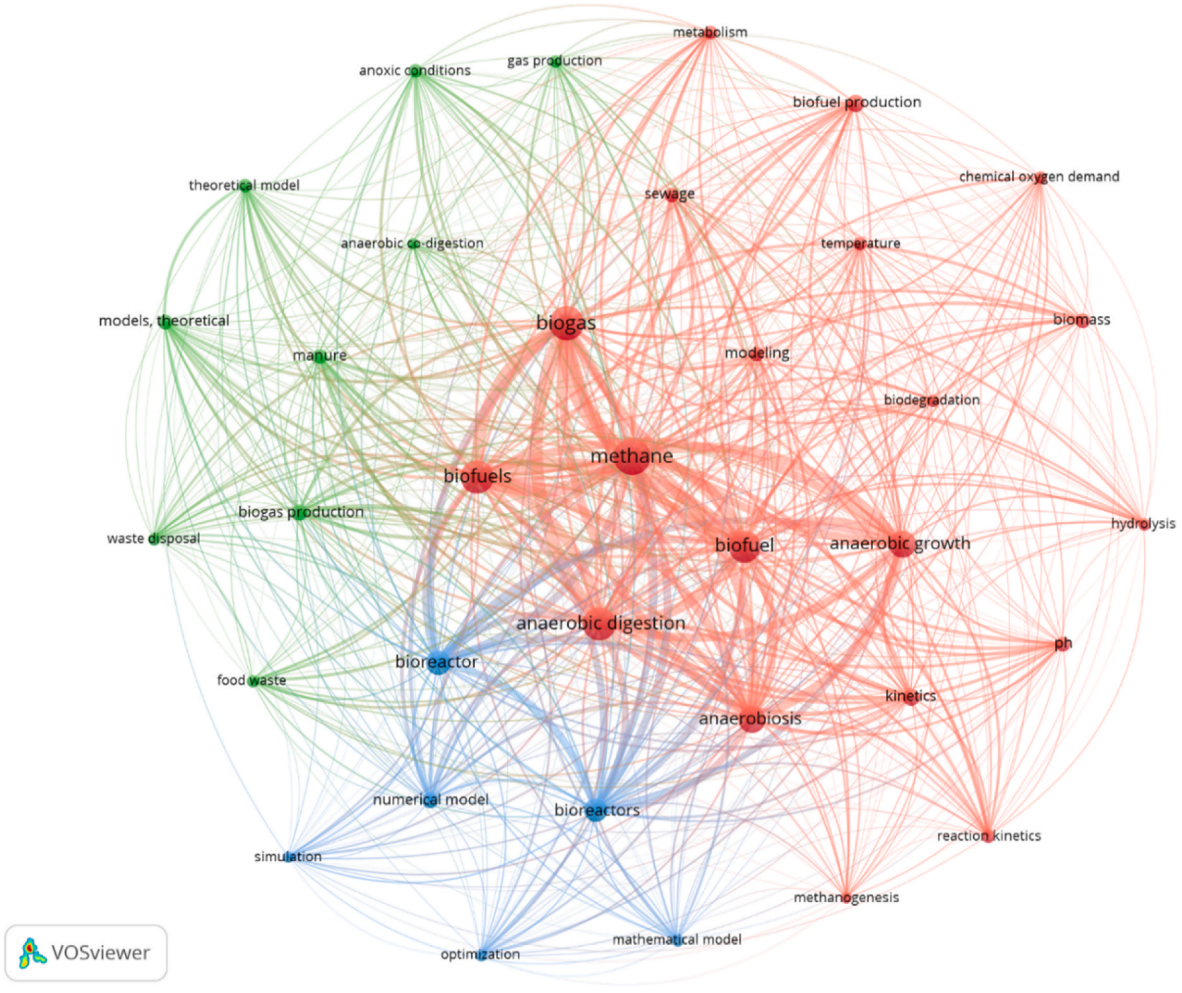

Fig. 1. Keywords co-occurrence network analysis using VOSviewer software.

Table 1
Summary of studies having ADM1 as the basis model framework to capture CH_4 output in a relevant environment or higher scale of operation.

Reference	Feedstock	Volume, m^3	Reactor type	Temperature, °C	Simulated parameters	Model extensions and modifications	Data analysis	Outcome
[27]	Primary and secondary sewage sludge	−0.16 −0.8	2-stage CSTR	35 and 55	Biogas (m^3/d) CH_4 (%), CO_2 (%), H_2 (%), Propionate (kgCOD/m^3), Acetate (kgCOD/m^3)	Two-stage AD and benchmark implementation to eliminate numerical discrepancies.	Parameter estimation	Successful parameter estimation and adequate prediction
[28]	Liquid manure and fodder for cows	3.5	STR	38	Biogas (Nm^3/d), CH_4 (%), CO_2 (%), H_2 (%), Propionate (mgCOD/L), Acetate (mgCOD/L)	Inflow fractionation		Able to predict biogas production and energy yield
[29]	Piggery manure and biowaste	−2 of 50 −2 of 91	4-chamber scheme	Mesophilic	Biogas (L/d), pH	Calibrated kinetic parameters		Appropriate for process design, optimization and predictions at serial reactors
[30]	1:1 primary and secondary sludge	10800	CSTR	Mesophilic	CH_4 (m^3/d), CO_2 (m^3/d), pH, TVFA (mg/L), TCOD (kg/m^3)	Stoichiometric coefficients expressing nitrogen release by the biomass decay process	Minimizing the sum of the squares between measurements and model values	Measurements agreed well with calculated model results
[31]	Grass silage	0.0312	2-stage CSTR	37	Biogas (L/d), CH_4 (L/d), CH_4 (%), TVFA (mg/L), TS-VS (%), pH	The liquid phase, gas phase, and acid-base equations to implement 2-stage AD		Good accuracy with experimental data
[32]	A blend of pig manure, wine, and gelatine	1.0	UASB–AF	Mesophilic	Biogas (m^3/m^3/d), CH_4 (%), CO_2 (%), H_2 (ppm), NH_4^+ (M), COD (g/L), Acetate (M), pH, HCO_3^- (M)	Addition of soluble fermentable substrates and calibration of acetoclastic ammonia inhibition		Successful validation for implementing new soluble substrates
[33]	Maize silage	0.24 and 0.5	2-stage	Mesophilic	Biogas (L/d, L/kgVS), CH_4 (%), CO_2 (%), H_2 (ppm), pH, Acetate (mg/kg), Propionate (mg/kg)	Estimated kinetic parameters	Residual sum of squares and estimation of parameter uncertainty	Confidence regions showed that the upper limits of the single hydrolysis rate constants were not bounded
[34]	Anaerobic sludge from cesspit	0.8	USAB	Mesophilic	Biogas (m^3/d & m^3/m^3), CH_4 (L/gCOD), pH, Effluent (kgCOD/m^3), Acetate (g/L)	Modeling sludge retention increases the external recycle		Average experimental data were within 10% of the simulated values
[35]	Municipal solid waste, grease trap sludge, and ley crop silage	4000	CSTR	Mesophilic	Biogas (Nm^3/d), pH	Parameters estimation	Index of agreement and normalized root-mean-square deviation	Good fit for biogas and NH_4–N. Low VFA and pH prediction accuracy
[36]	Primary sludge	6750	CSTR	Mesophilic	COD (g/L), CH_4 (m^3/d), Alkalinity (mg/L), VFA (gCOD/L)	Calibrated kinetic parameters		Default parameter can adequately characterize the sludge-based AD without the need for excessive experimental data
[37]	Wastewater from industries producing pharmaceutical and enzymatic products	1963	AGR – IC	35	CH_4 (m^3/d), CO_2 (m^3/d), H_2S (m^3/d), VFA (kgCOD/m^3), pH, COD (kg/m^3), SO_4 (kgS/m^3), NH_X (kgN/m^3), $H_XPO_4^{3-X}$ (kgP/m^3)	The fate of P and S compounds, physicochemical and ethanol reactions	Residual sum of squares	Relative mean error of 13–15%
[38]	Mixed primary and secondary sludge	10000	CSTR	Mesophilic	COD (kg/m^3), CH_4 (m^3/d), Alkalinity (mg/L), pH	Calibrated stoichiometric and kinetic parameters	Minimizing the root mean square error between experimental and model data	Measurements agreed well with calculated model results
[39]	A mixture of animal wastes	0.077	PABR	35	Biogas (L/L/d), COD (g/L), Acetic acid (g/L), Propionic acid (g/L), Butyric acid (g/L) pH, VSS (g/L),	Describe biomass retaining in the PABR		Adequate prediction considering the increased Solids vs Hydraulic Retention Time

(*continued on next page*)

Table 1 (*continued*)

Reference	Feedstock	Volume, m^3	Reactor type	Temperature, °C	Simulated parameters	Model extensions and modifications	Data analysis	Outcome
[41]	Glucose and syngas from straw pyrolysis	6.0	Up-flow	Mesophilic	CH_4 (L/d), H_2 (L/d), CO (L/d)	Modified Gas-liquid transfer process	ANOVA, sensitivity, and confidence interval analysis	High prediction accuracy with R^2 values above 0.86

However, the wider implementation is challenging because it is associated with some issues and constraints. For example, the production costs of biomethane are more expensive than natural gas [9] and especially, H_2 prices negatively affect process sustainability [10]. Moreover, operating strategies and proper reactor design can significantly increase CH_4 production capacity [11] that per se needs high gas inlet flows. However, increased proximity to gaseous feedstocks and especially, to cheap and green H_2 can fluctuate based on electricity prices [12]. Thus, the microbiome should be capable of adapting to rapid gas-loading changes.

Nevertheless, control strategies to predict the microbiome's ability to shift toward high production capacities are not yet exploited in an operational environment. Despite most of the research work has been focused on improving the lab-scale biomethanation, the technological readiness level of biomethanation was lately increased. Indeed, a number of groups around the world have already demonstrated the implementation of the biogas upgrading technology at a pilot-scale [13–17]. However, the published studies were mainly focused on the implementation of the process at a higher scale highlighting either the CH_4 production capacities or revealing insights on the microbial communities. On the contrary, modeling as means to predict, control and optimize the performance of gas fermentation on pilot or higher scale is rather scarce. Indeed, kinetic models were mainly applied to gas fermentations in lab-scale tests [18–20]. Pilot or higher scale studies were mainly putting attention on modeling the AD processes using liquid/-solid waste streams for biogas production. AD is a rather established technology and so, different model structures were evolved due to the need for predicting the process performance of digesters fed with agricultural or municipal wastes/wastewater. Due to the fact that AD systems are fed with inlets of alternating composition, at non-steady loading rates along with seasonal variations; there was a need to develop tools that can be useful for the plant operators in order to design feeding strategies, alleviate process instabilities and retain high system efficiency [21]. On this topic, BioModel and ADM1 are well-known model frameworks to understand, characterize, predict, and optimize AD processes. Multiple amendments, modifications, and additions occurred during the past years in both frameworks. Specifically, ADM1 was markedly improved –supported by the IWA Specialist Group on Modelling and Integrated Assessment –and utilized at different scales of operations from lab-to full-scale applications. On the other hand, BioModel has mainly been used in describing AD process at a lab-scale. Hence, fundamental knowledge was generated over the years from both model frameworks and the basic understanding of the AD process was improved.

This article aims to provide an overview of the two most used multistep dynamic AD models, namely ADM1 (for higher-scale applications) and BioModel (for lower-scale applications), and their role and amendments in supporting process development and decision-making in the bio-based gas production sector. A review of past practices, along with the benefits, barriers, opportunities, and challenges of introducing kinetic modeling to processes established at relevant scales is presented. Also, two case studies are simulated using the BioModel to explore its potential for higher-scale applications. Overall, it is discussed how these existing high-fidelity AD models can provide a basis to develop, predict, and finally support biogas and biomethanation processes at a larger scale.

2. Review methodology

Exploiting the Scopus database during the periods of 2010–2022, a sum of 154 articles was collected using the following keywords: biogas, biofuel, methane, and modeling. The relevant keywords analysis was conducted in the VOSviewer software. A minimum number of occurrences of a keyword was set to be 20 and subsequently, a network visualization was generated (Fig. 1). The color and size show the cluster and the occurrence frequency of keywords, respectively; while the lines connecting the circles indicate the links among keywords. Based on keywords, the collected articles were clustered as follows: 1) AD, biofuels, biogas, and methane (red cluster); 2) conditions, process parameters, and characteristics (green cluster); 3) engineering perspectives including reactors and modeling (blue cluster). The main keywords included AD, biogas, and biomethane production, and the impact of modeling to simulate and optimize AD reveals a trend for research and also, the need for further development in the area.

The keywords co-occurrence show that mathematical modeling of AD processes is still a small part of all the research focused on this area. This fact can be explained by a number of reasons, the main one being the difficulty in finding researchers who are simultaneously interested in biological processes and well-versed in mathematics and coding. Furthermore, graduate students tend to consider laboratory experiments more important than data analysis or learning writing skills [22] and often have fears and difficulties in learning a computer progamming language [23]. However, this scenario is bound to change, since there is a rising interest in advanced information technologies, artificial intelligence, and machine learning models which can make sense out of the increasing amount of data collected and provide reliable process monitoring and forecasting [24].

3. ADM1 applications on pilot- and full-scale case-studies

The initial ADM1, published in 2002 included 26 dynamic state variables, 8 implicit algebraic variables, and 32 dynamic concentration state variables implemented as differential equations [25]. Due to the need for reduced impreciseness and the complexity of the AD process, multiple attempts have been made at adding process reactions, state variables, stoichiometry-based relations, and kinetic parameters [26]. Compared to other complex model frameworks, ADM1 has been used to an increased extent in the literature for modeling and simulation of processes at pilot- and full-scale, respectively (Table 1).

Blumensaat and Keller [27] extended ADM1 applicability to a two-stage AD process, applying C and N balance checking. 'Benchmarking' implementation was used to validate the model accuracy developing a customized procedure to limit the range of estimated parameters. Testing procedures revealed the need to better close the balances of inorganic C and N released from biomass decay to avoid discrepancies between content in the biomass and availability in the feedstock. While the model accuracy was validated at two-stage pilot AD, they communicated the need for basic research on closing the inorganic C and N balances, and further validate model agreement with measurements.

While ADM1 is a model framework that is based on COD, research attempts have revealed the need for improved inlet characterization when recalcitrant substrates are used [27]. Lübken et al. [28] examined the usage of VS instead of COD and Weender analysis along with Van

Soest for the determination of carbohydrates, proteins, and fats. The improved inflow fractionation could better capture the biogas production trend using cattle manure and energy crops for different feeding intervals. As mentioned, ADM1 was built on a COD basis and focused on the AD of sewage sludge. The authors decided to use a VS basis in their study due to their experimental methodology and the usage of manure. The improved simulation was achieved because of the better influent characterization and not due to the change of basis. To improve the numerical accuracy of the model using different substrates, the need for calibrating the degradation and decay rates was highlighted [29]. Especially, the calibration of the coefficients for disintegration and decay rate for sugar degraders and the half-saturation constant for sugar was markedly different than the default parameters. The research highlighted the need for proper parameter estimation when ADM1 is used to describe the degradation of agricultural waste.

However, sludge characteristics can vary during reactor operation challenging ADM1 predictability. To minimize limitations from sludge variability, dynamic data from 150 days of operation of a full-scale AD plant was used to calibrate the ADM1 with a focus on N and C mass balances [30]. After calibration, the dynamic data of 215 days were used to validate the simulations of the modified ADM1. The amendments included the consideration of the inorganic nitrogen coming from biomass decay and the relevant stoichiometric coefficients. Calibrating the sensitive parameters (e.g. hydrolysis constants, uptake rates for sugar and selected VFA degraders, half-saturation constants for sugar and acetate degraders, yield coefficient for H_2-fueled archaea) led to improved model predictions.

Thamsiriroj and Murphy attempted to simplify the 2-stage AD of grass silage [31]. The initial differential system in ADM1 contained 32 and 3 equations in the liquid and gas phases, respectively. Thus, a 2-stage CSTR system demanded solving 70 ODEs. To reduce complexity to 60 equations, the number of variables and associated equations were decreased having only S_{H^+} (mole $H^+ L^{-1}$) as the sole state variable in the acid-base processes.

In another case study, the degradation of soluble fermentable organics (such as ethanol, glycerol, or lactate) was considered and followed glucose-equivalent reactions, while only the acetoclastic $K_{I,NH3}$ was modified compared to the original ADM1 values [32]. Co-digestion of liquid pig manure, wine, and gelatin was simulated showing that the applied methodology can be followed to implement more easily degradable substrates in ADM1. It is noteworthy that a pilot-scale UASB was used for biogas production. In such a system, intense recirculation secures a complete mixture in the liquid phase and thus, the modified ADM1 version was mainly used to explain the process outcome.

Carbohydrates contribute to a huge fraction of the lignocellulosic waste streams and in a modified ADM1 version of Lübken et al. [33], sugars in maize silage were split up into slowly and readily degradable fractions. A two-parameter analysis was used to define hydrolysis rate constants. Despite the model having a good compromise between model complexity and predictive abilities, a variation in VFA content was detected. Also, it is known that mono-digestion of lignocellulose can lead to low bioenergy production due to a shortage of trace elements. It was revealed that modeling attempts towards the understanding of the micro-nutrient impact on microbial activities are missing in the literature.

Data from a UASB pilot reactor was also used in another study [34]. To avoid discrepancies and better describe the process, the external recycle was increased to achieve a higher STR than the HRT. Thus, feedstock composition that can vary over time and SRT were the only calibrated variables keeping the rest of values according to the literature. The calibrated version lead to less than 10% deviation between practical and simulated data.

Nordlander et al. [35] compared the simulation output variables with data obtained from full-scale plant monitoring. To define the initial conditions, the plant was simulated for 5000 simulation days using an average of the input data. To improve the accuracy of the full-scale co-digestion plant, the hydrolysis rate coefficients were determined for all main substrates. Then, a sensitivity analysis was conducted to define the extra kinetic parameters that should be adjusted. While the AMD1 output was improved after calibration, the need for more frequent and better substrate characterization was revealed. Improved substrate characterization frequently can highly affect the prediction of the biogas process. In a comparative study, the ADM1 was calibrated using data from 200 days obtained from a sludge-based digester [36]. Nine kinetic parameters were calibrated by minimizing the sum of the squares of the weighted deviations between practical data and simulations. The model outcome was validated on long-term and dynamic operation data showing the good capability of predicting methane output.

The scalability of ADM1 was also assessed in data obtained from an anaerobic granular reactor with internal recirculation simulating a flow reactor model consisting of CSTR in series [36]. ADM1 was upgraded with the fate of SO_x^{2-}/H_xS^{2-x} fractions and $H_xPO_4^{3-x}/P_{organic,P}$ profiles and adding inhibition factors for ethanol degraders. H_2 uptake rates or H_2-degraders and K_s for acetate were modified to capture the competition between sulfate-reducing bacteria and methanogens. C and S balances showed satisfactory average deviations, a suitable explanation of gas-liquid mass transfer, and competition among bacteria and archaea for the same substrates. Despite the acceptable numerical accuracy, inhibition by VFAs and long-chain fatty acids was not considered. Furthermore, increased minerals in the inlet will subsequently increase the formed precipitates that will compete for space with the microbiome. Thus, more efforts are needed to address the observed limitations.

Similar to previously applied approaches in the literature, Ozgun calibrated the most sensitive parameters and then, validate the data at long-term operation (>1 year) of full-scale AD of sludge [38]. It was concluded that alkalinity can be used as a fast indicator to control AD due to its high sensitivity and a more dynamic profile than pH. Some discrepancies were observed in methane output and were attributed to sludge composition. Thus, the need for improved and regular inlet characterization was shown again.

To expand the usage of ADM1 at different reactor systems (i.e. PABR), Michalopoulos et al. [39] included a parameter to describe the difference between SRT and HRT. The examined pilot-scale PABR was operated at alternating feeding rates. The kinetic parameters were estimated at a specific period while the established model was used to validate a separate experimental phase as advised earlier [25]. The trends of VS, VFA, and pH had a satisfactory agreement with the experimental data. Some deviations were attributed due to inaccuracies between sampling time and switching periods. Overall, it was concluded that the model could predict the performance of a system operated at different SRT and HRT.

To account for the intracellular microbial activity Weinrich et al. [40] augmented the ADM1 by coupling the standard kinetic model to FBA models of specific methanogenic species, namely, *M. barkeri* and *M. maripaludis*. In the original ADM1, a yield coefficient is necessary to describe the impact of microbial activity on substrates and products. This is unnecessary in the coupled model for those steps which FBA models replace. Thus, their respective yield coefficients are no longer required as they are implicitly encoded in the topology of the species' metabolic network. The coupled model was tested in steady state and dynamic conditions when changing a constant feed of maize silage from continuous to pulsed feeding. The final average methane production remained very similar for both the standard ADM1 and the augmented ADM1 with FBA while both the initial response of the methanogenic population at the onset of pulsed feeding as well as its dynamics between pulses deviates considerably. In contrast to standard ADM1, the coupled model described the intracellular metabolic pathway activity in much higher detail. Overall, the augmented ADM1 with FBA models can provide a convenient tool to interpret time series data from operational biogas plants, explore theoretically possible maximal yields and process

efficiency, identify early warning signals of reactor failure, and test intervention strategies to avoid costly reactor breakdowns. Finally, a recent study extended the application of ADM1 to the co-fermentation of glucose with syngas [41]. The major modification included a detailed description of the gas-liquid mass transfer mechanism. Moreover, inhibition terms were added on butyrate/propionate/acetate degraders and acetoclastic/hydrogenotrophic archaea to describe CO inhibition at high partial pressures. The model was calibrated in lab data and validated at a 6 m^3 pilot-scale reactor. The modified version matched well the composition of CH_4 and H_2, while some discrepancies were observed for CO leading to decreased accuracy compared to the lab tests. The main reasons for deviations were primarily attributed to the composition of the fed gas (e.g. H_2S) and the simplification of the microbiome composition in the model. Nevertheless, the performance was well-captured indicating that the upgraded model can be used to forecast the performance and thus, optimize the syngas biomethanation.

4. Advances of BioModel

Historically, a dynamic model describing the AD of organic substrates was developed in 1993 by Angelidaki et al. [42] having as initial scope to describe ammonia inhibition. The initial model included 12 chemical compounds, 1 enzymatic hydrolytic step, and 4 bacterial steps. Subsequently, model complexity was enhanced to improve the description of the AD process focusing on diverse co-digestion strategies, process inhibition, and gas fermentation. It differs from the ADM1 in two main aspects: (i) it expresses substrate compositions in terms of volatile solids (which is considered more accurate in cases of organic wastes with a high concentration of solids) as opposed to the use of COD in the ADM1; (ii) it uses Monod-type growth kinetics as the reference for calculating conversions, instead of the substrate uptake rates (with implicit biomass growth) used in the ADM1. Despite these differences, however, the two models work largely the same [43], which points to their good interchangeability.

Despite BioModel being mainly validated in lab-scale experimentation, its applicability to full-scale data was also proved in one of the first studies. Specifically, the BioModel was first modified to incorporate 19 chemical compounds, 2 enzymatic processes for carbohydrates and proteins, and 8 microbial groups [44]. Initially, the numerical accuracy of the upgraded model was calibrated and validated during the co-digestion of manure with lipids or protein in lab-scale reactors. Subsequently, the performance of a full-scale plant operating under co-digestion of manure with lipids was also validated. The real-life data were fitted quite well, while some discrepancies were attributed to non-proper mixing of the reactor when the model considers a fully-mixed system.

Kovalovszki et al. [45] extended the BioModel applicability in co-digestion strategies by examining diverse substrates (i.e. manure, grass, food and garden waste, and sludge). Moreover, a detailed systematic methodology was developed and applied to estimate a general set of parameters for the co-digestion of a wide range of organic substrates and waste. The numerical accuracy was improved after applying the parameter estimation methodology and it was shown that a general set of 13 model parameter values can be used as starting point for diverse case studies.

Driven by the need for developing efficient power-to-X technologies, there was a significant progress lately in the field of biomethanation using external H_2. Lovato et al. [46] attempted to explain the phenomena of gas-liquid mass transfer and broaden the applicability to the in-situ biogas upgrading process. Indeed, the corresponding dynamic mass balance equations for H_2, CO_2, and CH_4 were upgraded considering the gas-liquid mass transfer mechanism, describing that the net transfer between the gas and liquid phases is determined by the concentration gradient, with the rate of transfer determined by the mass transfer coefficient and the surface area across which the mass transfer takes place. The BioModel has been extended with the hydrogenotrophic pathway and validated with two case studies showing the sensitivity to the H_2 injection rate.

Continuing the work on H_2-fueled communities, the SAO were consequently added to the model [47]. Specifically, the added H_2 can be channeled through homo-acetogenesis towards acetate accumulation which could be oxidized by SAO. To describe the dynamic interactions between acetoclastic and hydrogenotrophic archaea, the SAO group was also considered. Despite the methane and VFA trends were captured by the amended version, a big deviation was observed between the experimental and simulated butyrate concentrations. As explained, the accumulated butyrate should be originated from lactose fermentation (i.e. occurred in the first stage of the system) since cheese whey by-products were co-digested and also, from the high acetate levels which could have inhibited the syntrophic butyrate oxidizers.

An extra add-on to the BioModel was associated with metals' inhibition. Initially, an extra function was added to model the non-competitive inhibition of Na^+ to the acetoclastic methanogens during the co-digestion of saline substrates [48]. The Na^+ inhibition constant was estimated by fitting data from batch experiments and was then used as initial values to simulate continuous mode AD. The model indicated process dynamicity in qualitative trend and the incorporation of more microbial groups (e.g. propionate degraders) would be needed to achieve more accurate outcomes.

Apart from sodium, the effect of potassium as extra trace metal on AD performance was assessed [49]. In accordance with previous approaches to model the impact of metals, a non-competitive function on acetoclastic methanogens was introduced to fill this literature gap. The inhibition constant was estimated using data from the AD of municipal biopulp and sludge with an excess of potassium. The predicted methane generation was slightly lower compared to the experimental data. The finding was attributed to microbial adaptation to the new conditions highlighting the need for more research work in this area.

Kovalovszki et al. [50] examined the adaptation of the AD microbiome to temperature fluctuations. The function followed Arrhenius' principle and was based on the fact that a potential temperature increase can boost growth rates. However, the growth declines beyond an optimum value due to the denaturation of intracellular proteins. Adaptation time constants were added for the microbial groups implementing a delay function to model the impact on methanogens due to their higher sensitivity compared to bacteria. The modified multistep dynamic AD model had an improved qualitative indication of the performance of AD reactors facing temperature fluctuations. The work can serve as the basis for simulating the adaptation of microbial communities in other variables (e.g. pH, ammonia).

Furthermore, the impact of oxygen on the degradation of recalcitrant lignocellulosic substrates was also modeled [51]. The hydrolysis of wheat straw was modeled incorporating first-order kinetics adding a rate constant for the presence of O_2, while a non-competitive inhibition term was added to describe inhibition. The modified BioModel followed the trend of CH_4 generation and could describe the process in an approximate matter. Nevertheless, the amended version could not be used to design a clear strategy for establishing micro-aerobic conditions for increasing methane generation. Aerobic uptake can increase the redox levels stressing the methanogens and increasing the CO_2 levels in the biogas. More experimental data are needed to define the optimal levels, calibrate the BioModel and validate the accuracy.

As an inspiration for the microbial growth-modulating temperature-effect function, the prediction of Na^+ inhibition was further improved by adding a dynamic mathematical function to implement the adaptation of acetoclastic methanogens to the inhibitor [52]. Thus, the Na^+ inhibition constant was expressed as a function consisting of a long-term adaptation and a short-term dynamic growth response. The thresholds of adaptation to Na^+ were estimated in an AD system co-digesting macroalgae with manure and were further estimated and validated in a second case study using the same substrates. Through the applied methodology, error measures (i.e. mean error and weighted absolute

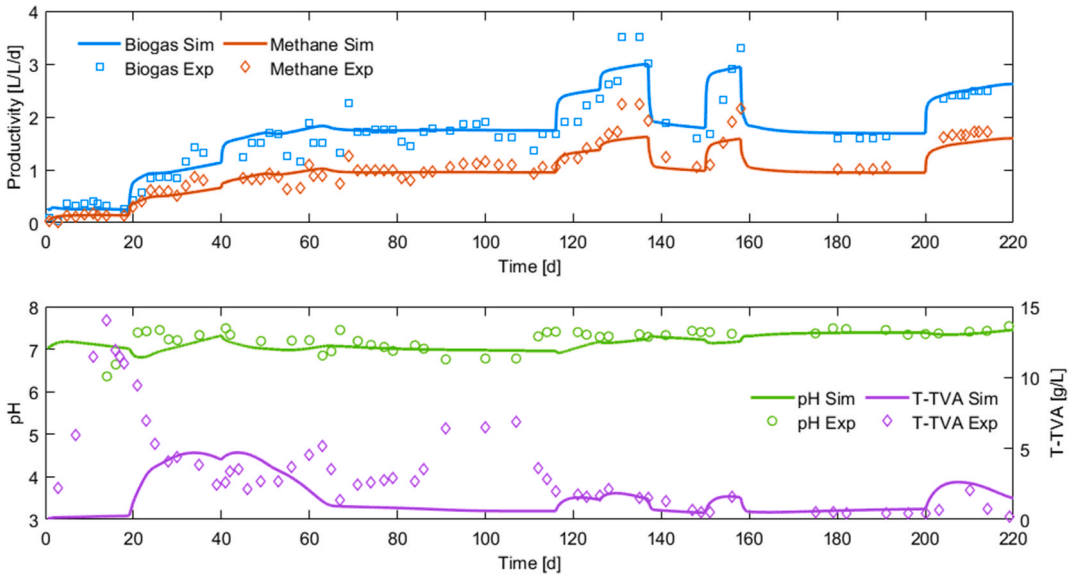

Fig. 2. Experimental data (markers) and Biomodel simulation (continuous lines) of pilot-scale AD reactor fed with municipal biopulp. Process demonstration in Avedøre WWTP [54].

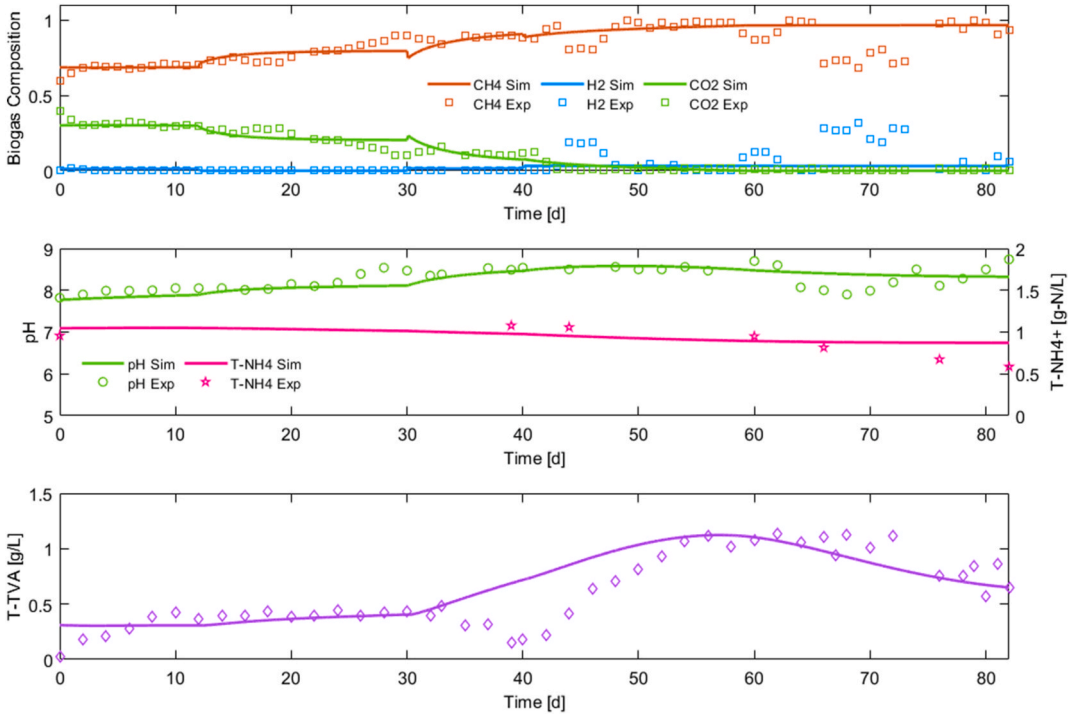

Fig. 3. Experimental data (markers) and Biomodel simulation (continuous lines) of pilot-scale trickle bed reactor fed with biogas and H_2. Process demonstration in Lemvig Biogas plant [13].

percentage error) were decreased and the simulations reached a good agreement with the experimental data. Towards further improvement, a deeper taxonomic characterization of the microbiome –for example, the existence of halotolerant methanogens in the inoculum –could enhance the accuracy of the simulations.

With a focus on microbial communities, Lovato et al. [53] attempted to describe the effect of invaded microbes to alleviate ammonia inhibition in AD reactors. SAO was added as an extra native microbial group. Native and bioaugmented groups were considered to have the same functions but different growth characteristics (e.g. growth rates, inhibition tolerance). To tackle ammonia inhibition, the importance of having a culture enriched in hydrogenotrophic methanogens was revealed. When added at high abundance, SAO can jeopardize the recovery of acetoclastic methanogens consuming most of the accumulated acetate. While the microbiome stress due to acetate is initially decreased, SAO can subsequently proliferate and consume more acetate for H_2 production. Thus, the biogas process is negatively affected in the long term. Overall, kinetic characteristics and composition of bioaugmented culture were crucial parameters to predict adequately the experimental trends.

Despite one of the first BioModel versions was applied in full-scale data, its applicability was not deeply validated and highlighted

Table 2
Summary of amendments in BioModel to simulate AD process.

Ref.	Feedstock	Volume, L	Reactor type	Temperature, °C	Simulated parameters	Model extensions and modifications	Data analysis	Outcome
[44]	Manure and industrial wastes	4 of 200000	CSTR	55	CH_4 (L/L/d), pH, VFA (g/L), FAN (g/L), Acetate (g/L), Propionate (g/L)	Calibration to better describe lipid- and protein-rich waste		Sufficient accuracy prediction during periods of critical changes
[45]	-Manure and meadow grass -Sludge, food, and garden waste	−3.5 −7.5	CSTR	Mesophilic and Thermophilic	Biogas (L/L/d), CH_4 (L/L/d), TVFA (g/L), NH_4^+ (g-N/L)	Parameter sensitivity analysis and estimation methodology	Stepwise parameter sensitivity analysis	Improved simulation accuracy at dissimilar case-studies
[46]	Cheese whey and manure	−1.0 −1.8	CSTR	55	Biogas (L/L/d), CH_4 (L/L/d), CH_4 (%), CO_2 (%), H_2 (%), pH, TVFA (g/L)	Addition of hydrogenotrophic methanogenesis Addition of H_2 in the gas feed for biomethanation	Latin Hypercube Sampling method for sampling. Sensitivity analysis through Partial Rank Correlation Coefficient method	Biogas content and H_2 uptake predictions with deviations below 10% compared to experimental data
[47]	H_2, cheese whey permeate and waste powder	3.0	2-stage CSTR	55	CH_4 (L/L/d), H_2 (L/L/d), Butyric acid (g/L), TVFA (g/L)	Incorporation of syntrophic acetate oxidizers		CH_4 and TVFA changes were well-captured at single- and two-stage reactor
[48]	Biopulp and macroalgae	7.5	CSTR	55	CH_4 (L/L/d), TVFA (g/L), pH	Non-competitive inhibition of Na^+		Unveil the impact of Na^+ inhibition on aceticlastic methanogenesis
[49]	Biopulp and sludge	1.8	CSTR		CH_4 (L/L/d), Acetic acid (g/L), Propionic acid (g/L), pH	Non-competitive inhibition of K^+	Coefficient of determination and root mean square error	Accurately predict the impact of K^+ inhibition on AD process
[50]	-Manure -Manure and meadow grass	−0.7 −1.8	CSTR		CH_4 (L/L/d), TVFA (g/L)	Implement a microbial temperature-dependent function	Root mean square error	Attractive tool for simulating AD processes facing temperature variations
[51]	Wheat straw	0.2	Batch	54	CH_4 (NmL/gVS)	First-order aerobic hydrolysis equation for complex carbohydrates	Minimization of square-error between the model output and experimental values	Qualitative indication of O_2 impact in the AD process
[52]	Manure and macroalgae	1.8	CSTR	54	CH_4 (L/L/d), TVFA (g/L), pH	Microbial adaptation to salinity	Mean error and weighted absolute percentage error	Reveal the potential existence of methanogens' tolerant to salinity
[53]	-Cattle manure -Glucose	−1.8 −0.35	-CSTR -Sequencing batch reactor	37	CH_4 (L/L/d), TVFA (g/L), pH	Alleviation of ammonia inhibition through bioaugmentation	Mean error, weighted absolute percentage error and mean absolute percentage error	Efficient and quick tool for examining different bioaugmentation approaches

through the years. To evaluate the numerical accuracy and applicability of the recent versions, simulations were conducted in the present study exploiting data from recently published pilot-scale experiments [13,54]. Regarding the first case study, Fig. 2 shows the simulations' outcome of a 500 L AD reactor treating biopulp from municipal bio-waste for 220 days [54]. Biogas and methane productivity and pH were well predicted, with RMSE under 20%. The trend for total volatile fatty acids prediction was also well simulated, however, there are notably two periods of instability that were not comprehended by the model: (i) the first 25 days of operation, which comprised the adaptation of the inoculum to the substrate and operational conditions - this kind of phenomena is not currently described by the BioModel and (ii) a malfunction of the heating system from day 53–69 which increased VFA concentration due to temperature fluctuations and facility maintenance during days 108–115. The metabolic intermediates decreased when the operation returned to normal and the stabilization was predicted by the model. Several operational modifications of the organic loading rate, which caused the fluctuations seen in the top graph of Fig. 2, were also correctly simulated.

Fig. 3 shows the experimental data and process simulation of a 68 L trickled bed reactor whose objective was to promote the ex-situ biomethanation of biogas from a previous reactor with H_2 from an external supply [13]. Digestate was also fed to the system to provide nutrients for the enriched consortium. Methane content in the outlet biogas and pH were remarkably well predicted, with RMSE below 12%. Total VFA simulation presented an error of 27%, but with a correct trend throughout the 82-day experiment. The amendments performed in the BioModel for gas-to-liquid (and vice-versa) transfer have proven to be robust to model in-situ and ex-situ biogas upgrading scenarios consistently.

Volatile intermediate acids prediction with very small deviations is still challenging. This is because there are a number of minor metabolic routes that are not covered by any model due to the increased complexity added to coding and computational time. However, they still exist and cause discrepancies. A few examples are the lactic acid degradation into propionate and acetate, ethanol degradation to acetate, and hexanoic, succinic, and malic acids degradation. This type of prediction could benefit from machine learning models that use data from full-scale plants. Nonetheless, the updated and extended BioModel (Table 2) replicates the dynamic behavior of the aforementioned variables well, making it a powerful tool for improved process design and selection of operational conditions.

Overall, the current BioModel has been updated with gas-to-liquid (and vice-versa) mass transfer mechanism, kinetic parameters and biochemical reactions for SAO and hydrogenotrophic pathways, and microbial adaptation to temperature and salinity. As "add-on" amendments, there is the biogas upgrading module, which covers in-situ and ex-situ biomethanation, and the bioaugmentation module.

5. Conclusions and perspectives

This review summarizes the application of the most commonly-used model frameworks as means to validate and optimize the AD processes. With the ongoing modifications over the years, both ADM1 and BioModel have proved their potential to be used as a practical and multi-purpose simulation tool in a wide range of applications at pilot- or full-scale. In general, high accuracy was achieved in most studies between experimental and model outcomes.

The various applications can provide hints and guidance to overcome barriers related to modeling. For example, the ADM1 is a powerful tool to predict the performance of wastewater-based AD and alleviate potential challenges, set the room for a better understanding of gas fermentation, and describe the fate of cations and anions that could promote the formation of precipitates inside the digested. To be noted that the above-mentioned solutions were applied in pilot- or full-scale case studies. On the other hand, BioModel was mainly used to describe lab tests and provide hints about common challenges or practices such as ammonia and cations inhibition, bioaugmentation, co-digestion, and adaptation to temperature fluctuations. To highlight BioModel's potential for implementation at a higher scale, two recently published pilot tests were successfully simulated herein. It is indicated that case studies of higher technological readiness levels can be also favored by this model framework.

The examined modeling frameworks have a great potential to expand the role of gas for Power to X and specifically, support the recent advances in the biomethanation area. To meet this target, high accuracy of experimental measurements is mandatory to succeed in close fits between the observed and simulated data. Proper characterization of feedstock, tools that can handle both gaseous and recalcitrant residual resources, and also, online measurements can further contribute to reducing the uncertainties. However, there are obvious gaps in the literature related to case studies focusing on gas fermentation. Limited research works are focused on the description of biological methanation at pilot- or full-scale using mathematical models and computational tools. Biomethanation using raw biogas and syngas fermentation are research hotspots that need further simulation and modeling efforts. Moreover, the impact of H_2S in the archaeal composition is not yet deeply modeled, while it is suggested that S compounds can have a positive or negative impact based on the concentrations. Furthermore, accurate measurements of CO_2 and H_2 concentrations in the liquid or gas phase are rarely available in the pilot- or full-scale plant operation due to the high cost of reliable experimental sets. Nevertheless, this imposes the need to account for reliable real time monitoring sensors. As highlighted FBA models can be incorporated in both modeling frameworks to gain more insights and detailed predictions on the intracellular activity of microbial species which are compatible with experimental measurements on enzyme synthesis activity or abundance, and metabolites interactions with specific microbial community members. This information has become available with unexampled detail through experimental advances in *meta*-transcriptomics, *meta*-proteomics, and metabolomics. Thus, it is paramount to account for reliable measurements that can highly improve model calibration and contribute to better predictions of methane production capacities during the pilot- or full-scale plant operation.

Last but not least, to verify the application range of these modeling frameworks -when these are updated with the addition of new amendments, and mechanisms, -it is a must to perform (i) a global sensitivity analysis of model inputs (e.g., influent composition) to model predictions including key performance metrics of the models (COD, total nitrogen, ammonia, TVFA, biogas productivity, etc.), and (ii) a global uncertainty analysis to propagate parameter and measurement uncertainty on model predictions, for subsequent optimization and scale-up studies.

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

No data was used for the research described in the article.

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