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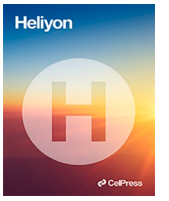

Research article

Modeling and forecasting biogas production from anaerobic digestion process for sustainable resource energy recovery

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ABSTRACT

Anaerobic digestion (AD) is one of the most extensively accepted processes for organic waste cleanup, and production of both bioenergy and organic fertilizer. Numerous mathematical models have been conceived for modeling the anaerobic process.

In this study, a new modified dynamic mathematical model for the simulation of the biochemical and physicochemical processes involved in the AD process for biogas production was proposed. The model was validated, and a sensitivity analysis based on the OAT approach (one-at-a-time) was carried out as a screening technique to identify the most sensitive parameters. The model was developed by updating the bio-chemical framework and including more details concerning the physico-chemical process. The fraction X_P was incorporated into the model as a particulate inert product arising from biomass decay (inoculum). New components were included to distinguish between the substrate and inoculum, and a surface-based kinetics was used to model the substrate disintegration. Additionally, the sulfate reduction process and hydrogen sulfide production have been included. The model was validated using data extracted from the literature. The model's ability to generate accurate predictions was testified using statistical metrics. The model exhibited excellent performance in forecasting the parameters related to the biogas process, with measurements falling within a reasonable error margin. The relative absolute error (rAE) and root mean square error (RMSE) were both less than 5 %, indicating a high ability of the current model in comparison with the literature. Additionally, the scatter index (SI) was below 10 %, and the Nash-Sutcliffe efficiency (NES) approached one, which affirms the model's accuracy and reliability. Finally, the model was applied to investigate the performances of the AD of food waste (FW). The findings of this study support the robustness of the developed model and its applicability as a virtual platform to evaluate the efficiency of the AD treatment and to forecast biogas production and its quality, CO_2 emission, and energy potential across various organic solid waste types.

1. Introduction

Recently, the world experienced rapid urbanization, accompanied by a significant expansion of the economy, industrialization, and

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human civilization. As a result, the global energy demand has increased, leading to a series of critical problems: the environmental impact (pollution, global warming, emissions of greenhouse gases) and the exhaustion of fossil fuel reserves owing to high consumption [1]. Consequently, the world faces the danger of climate change and the threat of an energy crisis, which could have damaging ramifications for the environment, human health, and the energy security of different countries [2]. These negative impacts have raised the awareness of the necessity to restrict the utilization of fossil fuels and shift towards energy sources that are safe, affordable, and sustainable [3]. The solution is to adopt an energy strategy focused on the realization of a transition to an environmentally friendly economy based on renewable energies by partially abandoning fossil fuels and evolving towards an energy mix that prioritizes green energies. Based on this, a considerable investment of efforts is essential in exploiting renewable sources and developing and optimizing the various conversion technologies to amplify their field of application in different sectors, particularly industry [4]. In this context, the valorization of biomass into energy represents a valuable source of bioenergy [5], playing a fundamental role in limiting the emission of greenhouse gases and contributing to sustainable development. In this optic, AD is one of the most efficient methods of exploiting a wide variety of biodegradable organic wastes [6] to produce a clean energy source known as biogas. It is composed of approximately 50–75 % methane (CH_4), carbon dioxide (CO_2), and other trace gases (nitrogen N_2, carbon monoxide (CO), and hydrogen sulfide (H_2S)), and is usually saturated in humidity [7]. Biogas is a polyvalent biofuel representing an ecological and economical option utilizable in numerous applications as fuel in cogeneration systems to produce electricity and heat [8] or purified by removing carbon dioxide and used as natural gas [2] or stored and used later to compensate the intermittency of systems based on solar and wind energy. Indeed, biomass's proportion of the global renewable energy sector is around 77 %, contributing nearly 10 % of the world's energy supply [7]. The International Energy Agency estimates that bioenergy will experience significant progress by 2030, and by 2050, this energy source could produce 30 % of the energy consumed in the world [9]. Consequently, AD technology represents a strategic and promising choice for advancing renewable energies [10], accompanied by biogas, which is a future sector worldwide.

Recently, AD has gained considerable attention as an advantageous option for treating organic waste [11]. The AD process is employed for treating a variety of waste types, including vegetable biomass [5], fish farm waste [12], fruit and vegetable waste [13], food waste [14], and agricultural waste [15].

Generally, the substrate used in the AD process can contain sulfur in various forms, such as sulfate, which during AD is reduced to hydrogen sulfide (H_2S) by the action of microorganisms called SRB (sulfate reducing bacteria) [16]. Concentrations of free H_2S close to 100 mg/L in the liquid phase inhibit almost 50 % of the methanogenic activity [17]. A high H_2S content in biogas leads to a corrosive effect that can severely damage the various equipment used in AD plants and energy conversion systems. In addition, during the combustion of biogas, the gaseous H_2S is transformed into sulfur oxide (SOx), which is detrimental to the natural environment and health [18]. In the case of CHP systems, the permitted H_2S concentrations must be between 200 ppm and 500 ppm to ensure stable, efficient system operation [18].

Anaerobic digestion is a naturally biological degradation process based on a series of biochemical and physical-chemical reactions performed by a complex ecosystem of microorganisms (microbiota) [8,19]. This ecosystem produces, consumes, and exchanges different components in an anaerobic environment [20] to gradually convert the organic matter into a biogas enriched in methane and a biofertilizer with a high mineral content [21]. The microorganisms involved in the various phases of the anaerobic digestion process vary according to their physiology, nutritional requirements, kinetics of growth, and sensitivity to the environment [2]. Clearly, the AD is a complex process microbiologically, operationally, and chemically [22], posing problems of stability and monitoring due to its sensitivity to changes in environmental conditions [19].

To understand the AD process, evaluate the quality of the biogas produced (in terms of CH_4 and H_2S levels) and its upgrading, and to develop optimized AD technologies, we necessitate the employment of a mathematical model, which will offer the possibility of simulating the biological system and acquiring information concerning its operation [20,23] and energy performance.

Various AD models came into development, and the most famous and extensively used is the mathematical model ADM1 [24].

1.1. An overview of literature

The Anaerobic Digestion Model n° 1 (ADM1) is a mathematical dynamic model developed by the International Water Agency (IWA) in 2002 [25]. Is a structured model that incorporates most of the biochemical and physicochemical processes involved in the anaerobic degradation of the organic substrates [26].

Initially, the ADM1 was intended for modeling the anaerobic digestion of sewage sludge at mesophilic or thermophilic temperatures, but subsequently, it has been extensively applied to a variety of substrates, as documented in several research studies. For instance,

Fezzani Boubaker and al. [27] have developed a version of the ADM1 model to simulate the anaerobic mesophilic co-digestion of olive mill wastewater (OMW) with olive mill solid waste (OMSW). The researchers introduced a non-competitive inhibition function that considers the inhibition of methanogens caused by high concentrations of VFAs. This inhibition function was included in the acetate uptake process. The results of validation step showed, that the ADM1 model was able to generate modest predictions concerning biogas production for the case of a concentration of 80 g COD/l and a 12-day HRT. Further, Fezzani Boubaker (2009) [28] focused on improving the co-digestion of OMW with OMSW by modifying the original basic structure of ADM1 by adding extensions representing the inclusion of phenolic compounds and the process of their degradation to benzoate and then acetate, with the use of non-competitive inhibition functions to consider the inhibitory effects of these compounds. The comparison of simulations with experimental data has shown that the enhancement of the ADM1 model allowed the generation of accurate predictions for the steady-state results of gas flow rate, and soluble phenol concentrations for various influent concentrations under mesophilic conditions. The inconsistencies gap observed between the model output and the experimental results related to the weak modeling of the

anaerobic digestion process.

Another application of ADM1 is the treatment of different types of industrial wastewater, such as effluent from the pharmaceutical industry, investigated by Recep Kaan Dereli and al. [29]. These Turkish researchers used the ADM1 model to simulate and analyze the experimental data from a laboratory-scale reactor (UASB) treating opium alkaloid wastewater under mesophilic conditions (35 °C). In the study, the disintegration process was applied just for the lysis of biomass and the fractionation of particulate COD, because of the high degradability and rapid hydrolysis of opium alkaloids in wastewater. The results of the validation phase indicated that the calibrated ADM1 model was able to predict experimental results for methane, and biogas flows with low accuracy for high OLR. The researchers observed that the precision of the model's prediction decreased with increasing OLR. In these conditions, the model simulated an overloaded situation while the reactor was operating correctly, leading to an overestimation of the biogas and methane flow values.

Moreover, the ADM1 model is also be used for modeling the DA of lignocellulosic biomass. For example, T. Thamsiriroj and al. [30] have utilized the ADM1 model to investigate the mono-digestion of grass silage in a two-stage wet process with recirculation of the liquor between 2 digesters in series. In the last 15 days of calibration, the average methane yield was estimated by the model with acceptable error compared to the experimental value.

In other studies, many researchers have chosen to use ADM1 to study the AD of organic waste. Haidong Zhou and al. [31] introduced a short modification into ADM1 model to explore the AD of different organic wastes (biowaste, cow manure, and corn silage) in mono-digestion and co-digestion. The study aimed to perform simulations to analyze the impact of variations in operating conditions of HRT, SRT, feeding time intervals, and input ratios of two substrates on biogas production from organic waste. Furthermore, the researchers implemented the ADM1 platform to develop and test a control system, which showed acceptable performance in maintaining methane flow and reactor stability.

Another feature is the ability of ADM1 to model the DA of a mixture of different substrates. For example, Katarzyna Bułkowska and al. [32] have used the ADM1xp model to simulate the co-digestion behavior of maize silage and cattle manure. The fit between model predictions and experimental data concerning biogas/methane production, pH, and VFA concentrations was evaluated using an objective function Jc. The value of Jc was high for biogas production due to its fluctuations during the experiment, which implied to the low ability of the modification of the model developed by the author's [32].

Besides, the ADM1 model was also applied in investigating the AD of agro-waste from agricultural activities. For instance, Jing Wang and al. [5] evaluated the AD and biogas production of vegetable biomass under high salinity and mesophilic conditions based on dynamic simulations of the ADM1 model and laboratory-scale experiments. The kinetic model was updated by incorporating oxalic acid and sulfate reduction reactions. The model was programmed and solved numerically by GPS X (process simulator) software and then calibrated using experimental data from two reactors operating with two different salts present in the soil.

Sunil Prasad Lohani and al [33], have used the ADM1 to model and simulate the AD process of domestic wastewater treated in an up-flow anaerobic sludge bed (UASB) reactor. The calibration of the ADM1 model and the evaluation of its applicability were made using experimental data from a pilot-scale UASB reactor operated in different HRTs and at variable loading conditions. Generally, the model generated estimations with an error of 10 % and showed a poor agreement with the experiment process. The validated model was applied to the analysis and the simulation of a real scenario concerning biogas production performance estimations for the University of Nepal's domestic wastewater treatment plant, pre-treated in a septic tank. The results of this study have demonstrated that the ADM1 model needs additional modifications to represent a powerful tool to predict the behavior of a realistically operating AD system and, consequently, its employability in the analysis of feasibility, design, and operation of WWTPs.

In a similar context of testing the applicability of the model to real plant systems, we cite the work of Piotr Biernacki and al. [33], who have evaluated the ability of the ADM1xp model based on the CHC approach to describe the productivity of an existing industrial-scale biogas plant, fed with a mixture of cattle manure and food waste. In their study, the researchers followed a pragmatic approach aiming to adjust only the disintegration kinetic constant for each substrate without evaluating the effects of the hydrolysis parameters (CHC approach). To test this approach, the researchers also adopted another ICH approach, which aimed to modify the hydrolysis parameters individually for each substrate. The comparison revealed that the ICH approach accurately predicted the total biogas produced with an error of 1.84 %, contrary to the CHC approach, which showed a very low predictive accuracy. The findings highlighted that a reduction in the adjusted parameters led to a lowering of the accuracy of the model simulation. This confirms that a correct characterization of the substrate and optimization of the most sensitive parameters of the model can improve the performance of the ADM1 and, consequently, its usefulness as a tool for simulating biogas plants.

Another benefit of the ADM1 model is the possibility to be applicable in modeling the start-up process, an important aspect to consider in the design of an AD system. In this context, A. Normak and his co-workers [34] have used an improved version of ADM1 to simulate the start-up of a pilot reactor fed with fresh cattle slurry. The improvements to the ADM1 model concerned the reformulation of the equation describing hydrolysis by integrating the Contois model and the function of inhibition of hydrolysis by VFAs and the addition of a new variable representing the concentration of inert gases in the headspace to represent the start-up phase accurately. The calibrated model showed good simulation results when it was tested in the case of a digester start-up fed with preconditioned cattle slurry. However, performing a detailed analysis of the substrate and inoculum, together with the calibration of sensitive parameters, will optimize the predictions of the ADM1 model, which will be able to provide valuable information on the self-start-up period and assist in predicting the total start-up time, as well as providing a better understanding of fluctuations in process parameters. The application of ADM1 in the study of the initial state of the digester can be a wise strategy in defining feed effluent characteristics to minimize the time needed to attain maximum biogas production.

The forecasting capacity of the original ADM1 model remains limited, as it does not consider many processes and components (exclusion of: precipitation/dissolution process of metal ions, sulfate reduction, trace elements …) due to the necessity to consider a

large number of parameters and components that will increase the complexity of the model.

These limitations have motivated various researchers to focus on modifying the basic structure of the ADM1 model to a more complicated form, to provide a more detailed description of the various mechanisms involved in the AD process, helping to optimize the model's prediction results.

Indeed, based on the standard version of the ADM1 model, numerous researchers developed modified versions for adapting the ADM1 to a specified application or modeling a defined substrate. One of the shortcomings of the original ADM1 model is that the dead biomass of all groups of degrading organisms is recycled to the composite particulate substrate X_C, to be treated again by the same disintegration process; this means combining two processes into a single process describing both the conversion of the substrate X_C and the generation of decomposition products, which is not the reality. In addition, the component X_I includes the inert products resulting from the disintegration (initial stage of DA) of X_C and the inert decomposition products (process carried out during DA); these two products have different nitrogen contents. This structure affects the evolution of the nitrogen content during the AD process, creating discrepancies in nitrogen conversion. To solve this kind of problem and improve the predictability of nitrogen release by the ADM1 model, the researchers B. Wett and al. [35] have introduced a new compound X_P representing inert decay products, produced with a factor of decomposed biomass. This modification distinguishes between biomass disintegration and decomposition processes, which weren't made in the original ADM1. The model was applied to the modeling of primary and secondary sludge at the laboratory scale, and it was able to describe adequately the experimental results. The model was implemented by ifak system (IFAK 2009, Germany) [32].

Additionally, we found studies that focused on the modification of the kinetic rates adopted in the model. For instance, Francis Mairet and al. [36] who have employed the original ADM1 model and a modified version based on the Contois kinetics for modeling hydrolysis steps to describe the AD of microalgae. The comparison between the two models showed that the modified version was able to describe accurately the experimental data except for the methane content, which was underestimated. This may be due to pH underestimation, as explained by the authors, who suggested that a detailed substrate characterization could improve pH and methane prediction. The findings of the study suggested that the ADM1 could be a valuable tool to represent the coupling of microalgae with anaerobic digestion processes and its optimization.

Other studies have focused on the addition of new components or processes. For example, Yang Zhang and al. [37], who have extended the ADM1 model by introducing several modifications: adjustment of the inorganic carbon and nitrogen balance to achieve equilibrium between carbon and nitrogen contents during AD, incorporation of inorganic phosphorus, and inclusion of the metal ion precipitation process. The simulations carried out by the modified model showed that the initial concentrations of calcium and magnesium ions and the change in the ratio of inorganic nitrogen and phosphorus affect methane production in the gas phase.

Luigi Franzo et al. [26] proposed a modified version of the ADM1 model able to simulate the complex dynamics of TEs precipitation and uptake in anaerobic conditions. The modified model takes into consideration the processes of precipitation and dissolution of trace elements (Ni, Co, and Fe) in AD; these processes were added in the form of new reactions of association/dissociation and precipitation/dissolution that takes account the interactions of trace elements with inorganic carbonate, phosphate, and sulfide. The simulations carried out using the modified ADM1 model showed the effects of trace elements and the initial sulfur-phosphorus ratio on pH evolution and therefor on the methane production rate.

For some substrate types, the original ADM1 formulation needs to be updated to take into account the complex nature of the substrate and its composition, which will contribute to improving the model's prediction results. For example, but not limited to, the study conducted by Poggio et al. [38], who have described the composition of the substrate as a function of new fractions to be included as new state variables in ADM1 to improve the prediction of methane production. Indeed, they proposed a novel methodology for fractionating solid organic substrates into particulate and soluble fractions based on a combination of a biochemical approach based on elemental analysis of the substrate and a kinetic approach based on data from bioreactor experiments. Based on batch data, the researchers found that the best fractionation model for green waste was that which included a particulate and a soluble fraction (model XS, with rAE = 4.3 % and R2 = 99.1 %), whereas, for food waste, two particulate fractions were necessarily recommended (model XX, with rAE = 3 % and R2 = 99.4 %). The results of the validation step revealed the ability of the modified model to generate good predictions for methane-specific yield, total and volatile solids, ammonia, and alkalinity, but was less precise for predicting methane instantaneous flow rate, pH, and VFA. This issue may arise due to several factors, including the inherent limitations of the ADM1 model, which does not account for various processes that can influence pH and methane production, such as sulfate reduction and solids precipitation. Additionally, reliance on default values for most ADM1 parameters is often inaccurate, as these parameters can vary depending on the substrate's nature and operational conditions, such as inhibition parameters. Furthermore, the experimental conditions and methods used, particularly for measuring pH and alkalinity, can result in low-quality data.

The application and modification of the ADM1 model have been carried out through its implementation and coding in various computer programs such as: i) AQUASIM 2.1 [39], ii) SIMBA [40], iii) MATLAB [26], iv) Phyton [41], v) Julia Programming Language's [42], and Aspen Plus [43].

1.2. Research context and objectives

From the literature, it is clear that the ADM1 model has proved to be a valuable tool for simulating the anaerobic digestion of a wide range of organic wastes, supporting the design and management of industrial plants, and predict system behavior under different operating conditions. In addition, the ADM1 model can constituting a common platform offering the opportunity to refine the basic structure of the model to adapt it to a given substrate or specific application.

Consequently, the high performance of ADM1 in modeling AD encouraged us to develop a modified mathematical model to cover

part of the gaps found from research in the literature; in order to improve understanding and optimization of the AD process.

From the literature, it has been noted that:

- In the studies (mentioned above), most of the substrates used in AD are composed of a particulate fraction that has not been considered in modeling the process.
- During modeling, substrate and inoculum were represented by a single variable (Xc) in the ADM1 model input. The two compounds have different characteristics, which need to be considered separately, especially when modeling AD with data from experimental experiments.
- In the modified version of ADM1 (ADM_xp) developed by Wett and al. [35], the fraction of biodegradable products resulting from biomass decomposition is recycled to the Xc component, which takes into account substrate and inoculum without distinction between them.
- Predicting and validating the transfer of H_2S to the gas phase has been the subject of limited research, despite its importance in the anaerobic conversion of organic waste.

In this context, the model has been modified and extended to consider:

- The difference between the influent (substrate) and the inoculum, as being two compounds with different characteristics, will be represented by two separate variables in the model.
- The effect of particle size by using surface-based kinetics to accurately model the disintegration process of organic waste, as suggested by Esposito and al. [44].
- That inoculum decomposition during AD leads to the formation of a fraction of biodegradable products, which are recycled another time to the inoculum, and an inactive inert particulate fraction represented separately by X_P, as proposed by Wett et al. [35].
- The extension proposed by Batstone [16] for modeling the sulfate reduction process as a simple method for predicting the levels of H_2S expected to be produced in the case of AD of organic waste containing low sulfate concentrations. It will enable an initial evaluation of biogas quality and its suitability for use as fuel for CHP systems.

Furthermore, we provide a comprehensive validation and calibration framework for our model, drawing on experimental data from a variety of AD investigations. We demonstrate the accuracy and dependability of our model across multiple operating circumstances and feedstock compositions using rigorous validation against experimental data, increasing confidence in its prediction capabilities. The modified model can allow for a more accurate assessment of system behavior and the adjustment of operating parameters to improve process efficiency.

Accordingly, this study seeks to achieve several goals, notably:

- Process understanding: modelling provides a better knowledge of the mechanism and reactions taking place in AD. It includes identifying the different stages of the process, the microbial species involved, and the key parameters and factors that influence biogas yield.
- Performance forecasting: using equations and mathematical functions, the model can predict the performance of the AD system. Including the volume of the biogas produced, the methane production rate, reaction time profiles, and more. These predictions are fundamental in estimating the economic viability and sustainability of the process.

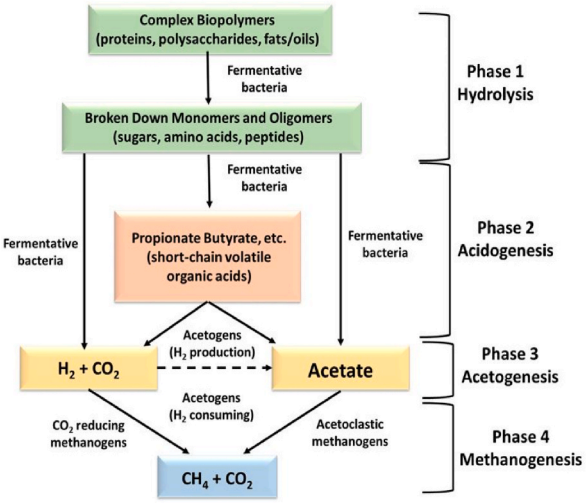

Fig. 1. The phases of the anaerobic digestion process [47].

- Process optimization: the modified model can serve as a tool to optimize the various parameters especially in determining the most favorable conditions of temperature, pH, carbon/nitrogen (C/N) ratio and organic load to maximize biogas production.
- Cost reduction and environmental impact: through optimization of the biogas production process, we can improve overall efficiency and also cut operating costs. Additionally, the model has the ability to predict the greenhouse gas emissions associated with biogas production and to identify the means of minimizing the environmental impact.
- Planning and conception of new installations: the model also allows the designing new AD plants based on site-specific parameters and the availability of primary feedstock. That facilitates preliminary planning and adapting the process to the local environmental conditions.

In summary, our paper represents a significant advancement in the modeling of AD systems independently to the type of digester and mode function, offering a more comprehensive, dynamic, and user-friendly tool for understanding and optimizing the biological process of AD. By addressing key limitations of existing models and incorporating novel features, our study suggests that the modified model can contributes to the advancement of both academic research and industrial practice in the field of anaerobic digestion.

2. The anaerobic digestion process

Anaerobic digestion is performed according to a succession of five phases (Fig. 1):

- Hydrolysis phase, also called solubilization [45], where proteins, lipids, and carbohydrates are decomposed into simple monomers (amino acids, LCFAs and simple sugars) by extracellular enzymes [13].
- Acidogenesis or fermentation process, where the products of hydrolysis are degraded into volatile fatty acids (VFAs) (such as acetate, butyrate, and propionate) with the production of hydrogen (H_2), alcohol and carbon dioxide (CO_2) [2].
- Acetogenesis or anaerobic oxidation, during which VFAs (propionate and butyrate) and alcohols are oxidized to acetate, dihydrogen, and carbon dioxide [2].
- Methanogenesis process, which is divided into two sub-processes. The first process is acetoclastic methanogenesis, based on the cleavage of acetate to methane and carbon dioxide [46]. This pathway is considered the predominant acetate degradation pathway in the mesophilic condition and is responsible for producing approximately 70 % of the total methane in the AD process [47,48]. The secondary pathway is hydrogenotrophic methanogenesis, using hydrogen and carbon dioxide to form methane [22]. This process produces nearly 30 % of the total methane in AD [49].

The AD process can be performed under three temperature conditions: psychrophilic (< to 25 °C), mesophilic (between 25 °C and 40 °C with an optimum temperature between 35 °C and 37 °C) and thermophilic (between 45 °C and 64 °C with an optimum of 55 °C) [13,48].

Various physical and operational parameters affect the development of AD and its performance [50], such as:

- The temperature inside the anaerobic digestion system which plays a crucial role in the growth of the bacteria and their activity.
- The pH levels that vary according to the quantity of the chemicals produced and consumed in the reaction environment [12]. A neutral pH is preferable for AD, ranging from 6.8 to 7.2 [51].
- The organic loading rate, considered an essential parameter for the design of the digester [52], given its influence on the various biochemical mechanisms in the process and influences biogas production [51,53].
- Agitation, an important parameter in the operating conditions for the digester [10,54], that can impact the efficiency of AD by influencing biogas production and energy consumption [55].

On the other hand, the physicochemical conditions of the reaction environment during AD are critically affected by the inhibition parameters, that can disrupt the microorganisms [49] and limiting or even halting their activities [50], leading to the process failing [49] in critical situations. Inhibition and toxicity factors include:

- Hydrogen sulfide (H_2S): at levels above 800 mg/L, it is a toxic component for methanogens, and can lead to the cessation of methane production.
- Light metals (Na, Ca, K and others): excessive quantities cause cell dehydration.
- P_{p,H_2}: in abundance can inhibit acetogenesis reactions. The partial pressure of dihydrogen must be under (10^{-4} atm) [56].
- NH_3: a toxic agent capable of penetrating cell membrane. It is an inhibitor that affect microbial activity, particularly acetoclastic methanogens.
- Heavy metals (Co, Zn, Cu and others): high concentrations damage the enzymatic function and structure of bacteria.
- Volatile Fatty Acids (VFA): concentrations exceeding 10 mg/L inhibit the growth of methanogens.

3. Materials and methods

3.1. Basic physical model structure of AD process

3.1.1. Biochemical framework

The ADM1 models the bio-chemical process by the inclusion of two phases:

- **The extracellular steps** incorporate disintegration as the first non-biological phase of AD, followed by the enzymatic hydrolysis phase [23]. These phases are modeled by the first-order kinetics described by equation (1) [39]:

$$\rho = k_{dis,hyd} \times X_{dis,hyd} \tag{1}$$

ρ: is the rate of disintegration or hydrolysis of the substrate (Kg COD/m^3).
$k_{dis,hyd}$: the kinetic parameter of hydrolysis or disintegration (d^{-1}).
$X_{dis,hyd}$: the concentration of the particulate substrate (Kg COD/m^3).

- **The intracellular steps** include acidogenesis, acetogenesis, and methanogenesis [37]. These phases are described by Monod kinetics based on substrate uptake, related to biomass growth [57], and expressed by equation (2) [39]:

$$\rho = k_{m,i} \times \frac{S_i}{K_{S,i} + S_i} \times X_i \times I \tag{2}$$

i: su, aa, fa, va, bu, pro, ac, h_2.
$k_{m,i}$: is the Monod's maximum specific absorption rate for the substrate i (Kg COD substrate/Kg COD biomass).
S_i: concentration of substrate i (Kg COD substrate/m^3).
X_i: biomass concentration i (Kg COD biomass/m^3).
$K_{S,i}$: the half-saturation value (Kg COD/m^3).
I: the inhibition functions.

The biomass death rate was modeled using a first-order equation (3):

$$\rho = k_{dec} \times X_i \tag{3}$$

k_{dec}: first order decay rate (d^{-1}).

Fig. 2 shows the structure of the biochemical phases in the ADM1 model.

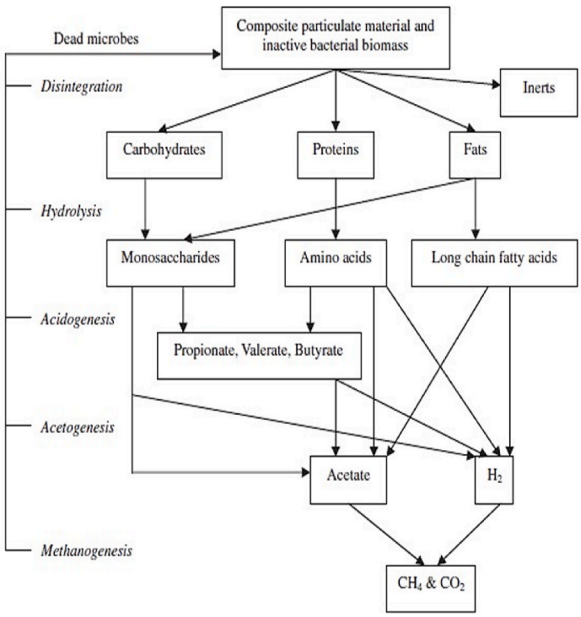

Fig. 2. The steps of the AD process in the ADM1 model [30].

3.1.2. Physicochemical framework

It represents all the non-biological reactions characterizing the various mechanisms and physicochemical exchanges inside the AD system. The modeling of physicochemical transfers is fundamental in determining and estimating different parameters, such as pH, alkalinity, biogas flow rate, and methane production [39].

- *Liquid phase equations:*

The dynamic evolution of the state variables of each component present in the liquid phase, is described by the following equations (4) and (5) [27]:

For soluble matter S:

$$\frac{dS_{liq,i}}{dt} = \frac{q}{V_l}\left(S_{in,i} - S_{liq,i}\right) + \sum_{j=1-19} \rho_j \nu_{i,j} \; ; i = 1-12 \tag{4}$$

For particulate matter X:

$$\frac{dX_{liq,i}}{dt} = \frac{q}{V_l}\left(X_{in,i} - X_{liq,i}\right) + \sum_{j=1-19} \rho_j \nu_{i,j} \; ; i = 13-24 \tag{5}$$

q: the inlet and outlet flow rates of the digester (m^3/d).
$S_{in,i}$: the entry concentration of soluble component i (Kg.COD/m^3), except for inorganic carbon IC and inorganic nitrogen IN (kmol/m^3).
$X_{in,i}$: the input concentration of the particulate component and biomass i (Kg.COD/m^3).
$S_{liq,i}$: the concentration of the soluble state variable.
$X_{liq,i}$: the concentration of the particulate state variable and biomass.
$\sum_{j=1-19}\rho_j \nu_{i,j}$: this term refers to the sum of the kinetic rates ρ_j for each process j multiplied by $\nu_{i,j}$ the stoichiometric coefficient determined from the Gujer matrix.

Acid-base equations:

The ADM1 model incorporates the following acid/base pairs: acetic acid/acetate, propionic acid/propionate, butyric acid/butyrate, valeric acid/valerate, carbon dioxide/bicarbonate (HCO_3^-), ammonium/ammonia [26]; which are deployed to describe the acid-base equilibrium. The kinetic acid/base reaction rates are calculated according to formula (6):

$$\rho_{A/B,i} = k_{A/B,i}\left(S_{liq,i^-} \times \left(K_{a,i} + S_{H^+}\right) - K_{a,i} \times S_{liq,i}\right) \tag{6}$$

$\rho_{A/B,i}$: the production rate of base B from acid A for component i.
$k_{A/B,i}$: the kinetic parameter A/B for the acid of component i.
S_{H^+}: the hydrogen ion concentration.
$S_{liq,i}$: the total concentration of the free form of the component I in the liquid phase.

The pH evolution during the AD process is determined from the concentration of dihydrogen ions, calculated based on the charge balance equation expressed by formula (7):

$$\sum S_{cat^+} + \sum S_{an^-} = 0 \tag{7}$$

The pH is calculated using the following expression (8):

$$pH = -log_{10}\left(S_{H^+}\right) \tag{8}$$

- *Gas phase equations:*

The modeling of the liquid-gas transfer process is extremely useful for predicting the energetic performance of the AD system, in terms of biogas quality and the rate of methane production.

The conversion of methane (CH_4), carbon dioxide (CO_2), and dihydrogen (H_2) into gaseous form is modeled by the dynamic equation representing the concentration of the gaseous dynamic state variable based on equation (9):

$$\frac{dS_{g,i}}{dt} = -\frac{q_g}{V_g} S_{g,i} + \rho_{T,i}\frac{V_l}{V_g} \; ; \;\; i = CO_2, CH_4 \; et \; H_2 \tag{9}$$

$S_{g,i}$: the concentration of the gaseous component in the liquid phase.
q_g: biogas flow rate (m^3/d).
V_g: the gas volume in the digester (m^3).

The mass transfer of these components from the liquid phase to the gas phase is modeled using the dynamic equation for the gas transfer rate [23], based on equilibrium between liquid and gas phase. The rate equation is expressed using formula (10):

$$\rho_{T,i} = k_L a \left(S_{liq,i} - K_{H,i} \times p_{g,i} \right) \tag{10}$$

i: H_2, CH_4 et CO_2.
$\rho_{T,i}$: the specific mass transfer rate of the gas i.
$k_L a$: the liquid-gas transfer coefficient (d^{-1}).
$S_{liq,i}$: the concentration of gaseous component i in the liquid phase corrected by factors 16 and 64 for H_2 and CH_4 (respectively) to account for their COD.
$p_{g,i}$: the partial pressure of the gaseous component i in bar calculated from the ideal gas law.

The biogas production rate (flow rate) is determined according to equation (11), as follows:

$$q_{gas} = k_p \left(P_{gas} - P_{atm} \right) \times {P_{gas}}/{P_{atm}} \tag{11}$$

k_p: the pipe resistance coefficient ($m^3.j^{-1}.bar^{-1}$).

3.2. Development of the modified model

In the present study, the basic structure of the ADM1 model described previously has been updated by adding new components and processes to enhance the quality of the model's numerical simulation results. The modifications applied to the model relate to:

3.2.1. The distinction between substrate and inoculum

In the original ADM1, the organic matter inside the digester is described by the state variable X_C, which refers to the particulate composite material undergoing the various stages of AD for biogas production. The ADM1 model does not distinguish between the substrate (organic matter) and the inoculum, which represent two components present in the digester possessing different characteristics, requiring them to be considered separately and not characterized by the same variable [58]. Consequently, the model was modified to incorporate two new state variables to individually characterize the substrate (X_{C_sub}) and inoculum (X_{C_inoc}), each processing experiencing a different disintegration process.

The disintegration of the inoculum was modeled by first-order kinetics ($\rho_{1\text{-}inoc}$), following the original ADM1. The disintegration of the substrate was modeled by surface-based kinetics ($\rho_{1\text{-}sub}$), which takes into account the effect of substrate particle size by the introduction of the parameter a* for a more accurate description of microbial substrate decomposition, especially in the case of solid organic waste (for example food waste) [59]. The expression for the substrate disintegration rate is the following (12):

$$\rho_{1-sub} = k_{dis,sub} \times a^{*} \times X_{C_{sub}} \tag{12}$$

The parameter a* represents the overall surface area of the organic particles to be disintegrated per unit mass (m^2/kg) [44], calculated using the following equation (13) [44]:

$$a^{*} = \frac{3}{\delta \times R} \tag{13}$$

with: δ is the density of the substrate (kg/m^3) and R is the radius of the substrate particles (m).
The term $k_{dis,sub}$ is the specific rate of surface disintegration, which depends on the nature of the substrate [44].

3.2.2. The separation between biomass decomposition and disintegration

In the original ADM1, the state variable X_C is used to simultaneously describe the conversion process of the feed substrate and the recycling process of the decomposed (dead) biomass products generated during AD. To differentiate between the two processes of disintegration and decay, we have introduced the change proposed by Wett and al. [35], which consists of integrating a new compound X_P representing the inert particulate products arising from biomass decomposition.

Wett and al. [35], have stoichiometrically described the distribution of the resulting dead biomass into a biodegradable fraction recycled in X_C and a non-biodegradable fraction represented by X_P.

The new change reported in our study is the consideration that:

- The biodegradable products of the biomass decomposition feed the inoculum (X_{C_inoc}), to be distributed between X_{ch}, X_{li} and X_{pr}.

- The compound X_P proposed by Wett and al. [35], stands for the accumulation of the inactive particulate fraction resulting from biomass decomposition (inoculum), depending on a decomposed biomass factor f_p.

3.2.3. The inclusion of the sulfate reduction process

The modeling and simulation of the sulfate reduction process in AD is an absolute necessity, enabling the prediction of the evolution of the H_2S concentration and its influence on the stability and productivity of the anaerobic process. This will allow a more comprehensive analysis of the system and a clearer understanding of its operation, notably in the case of preliminary studies for large-scale installations.

a. Description of the biological sulfate reduction process:

Sulfate reduction can be described according two different methods, depending on the concentration of sulfate in the substrate feeding the digester.

In our study, we have chosen to adopt the approach proposed by Batstone for modeling sulfate reduction, as an appropriate method for initially predicting H_2S concentration in the liquid and gaseous phases, in the case of wastes with a SO_4^{2-}/COD ratio of less than 0.1 (substrate with low sulfate concentration) [16].

In the extension proposed by Batstone [16], the soluble sulfate is reduced to H_2S, HS^-, and S^2 in the liquid phase by the intervention of SRB bacteria which use hydrogen as an electron donor (X_{hSRB}) (oxydation of available hydrogen) under anaerobic conditions, according to the reactions below (14)–(15):

$$4H_2 + H_2SO_4 \rightarrow H_2S + 4H_2O \tag{14}$$

$$4H_2 + SO_4^{2-} + H^+ \rightarrow HS^- + 4H_2O \tag{15}$$

S^{2-} was excluded from the model (neglected), as the simulated pH values before adding the extension were within the neutral range, where S^{2-} is present in low amounts.

b. Kinetics of the sulfate reduction process:

The inclusion of this new process, implied the integration of three new state variables: SIS (total reduced sulfides), SO_4^{2-} (sulfate), and XhSRB (sulfate-reducing bacteria).

The process of sulfate reduction is described by the uptake rate of hydrogen by hSRB bacteria. The rate equation for this process is modeled by Monod-type kinetics, including sulfate concentration (electron acceptor) and dihydrogen concentration (electron donor), according to the following formula (16):

$$\rho_{\text{uptake},hSRB} = k_{m,hSRB} \times \frac{S_{h_2}}{(K_{S,h_2} + S_{h_2})} \times \frac{S_{SO_4}}{(K_{S,SO_4,hSRB} + S_{SO_4})} \times X_{hSRB} \times I_{H_2S,inhibition} \times I_{pH,hSRB} \tag{16}$$

During AD, sulfate-reducing bacteria (SRB) in the anaerobic environment can inhibit the methanogenesis process by two mechanisms. The first is the production of H_2S, which represents a toxic component when it is present in the free form in the liquid phase, due to its ability to diffuse across the cell membrane, adversely affecting the growth of methanogens and thus perturbing the process of methane production [60,61]. The inhibitory effect of H_2S in undissociated form on hydrogen-consuming microorganisms, was modeled by a non-competitive function based on the following equation (17):

$$I_{H_2S,H_2} = \frac{1}{\left(1 + \left(\frac{S_{H_2S}}{K_{I,H_2S,H_2}}\right)\right)} \tag{17}$$

The second mechanism of inhibition is the competition between X_{hSRB} and the hydrogenotrophic methanogens for hydrogen, which represent the common substrate, used as electron donors simultaneously utilized by the two groups of anaerobic microorganisms in their growth and the elaboration of various products, such as methane [17,60].

In addition, pH inhibition on hSRB bacteria ($I_{pH,hSRB}$) was considered, and modeled analogously to the empirical function for pH inhibition for acetate, hydrogenated amino acids, in the original ADM1.

Concerning the acid-base equilibrium process, the new acid/base pair H_2S/HS^- was added to the model. The production rate of H_2S from HS^- has been calculated by the following equation (18):

$$\rho_{A/B,H_2S} = k_{A/B,H_2S}\left(S_{liq,HS^-} \times \left(K_{a,H_2S} + S_{H^+}\right) - K_{a,H_2S} \times S_{liq,IS}\right) \tag{18}$$

The charge balance was also update, by inserting sulfate ions SO_4^{2-} and hydrogen sulfide ions HS^- to consider their impact on the pH.

Concerning the gas transfer process for H_2S, it was modeled according to the gas transfer rate equation based on Henry's law used in the original ADM1, expressed as follows (equation (19)):

$$\rho_{T,H_2S} = k_L a \left(S_{liq,H_2S} - K_{H,H_2S} \times p_{g,H_2S}\right) \quad (19)$$

Finally, the decomposition of hSRB bacteria was modeled by a first-order equation (20) conforming to the ADM1 model.

$$\rho_{decay,hSRB} = k_{dec,hSRB} \times X_{hSRB} \quad (20)$$

The insertion of this process will allow the prediction of H_2S concentrations in the biogas and consequently evaluate preliminarily the quality of the biogas and determine its suitability to be directly valorized or will require an H_2S removal process (by specific methods) for reaching the target values.

The diagram of the biochemical transformations involved in the modified model is depicted in Fig. 1 (See APPENDIX A), and expressed by a modified Gujer matrix represented in Table 1 (See Appendix A).

3.3. Sensitivity analysis

An important aspect to consider when verifying the model's applicability in full-scale studies is to assess how the different parameters of the model impact the quality of its results. This will ensure a correct estimation of the parameters and consequently reduce model complexity and optimize the predictivity of the model.

In this context, the sensitivity analysis represents a useful technique for determining the contribution of each parameter of the model to the results; in other words, it enables a quantitative assessment of how a change in the value of an input parameter (perturbation) will affect the model's output [62]. Sensitivity analysis can be performed in two different modes: locally or globally [62].

In our study, a local sensitivity analysis (LSA) based on the one-at-time approach (OAT) was performed as a screening technique to classify the model's input parameters in order of importance by quantitatively evaluating the individual influence of each parameter on the model's result (output).

In our case, the mean methane production has been chosen to be the model output to examine as an important variable in the optimization of the anaerobic process.

Within the framework of this method, the input parameters were changed individually by increasing the value by 50 % while keeping the rest constant. The aim was to study the influence of parameter modification on the behavior of average methane production and thus determine the factors to prioritize in optimizing the model and those that can be fixed due to their low effect on the results.

The dependence of the model's parameters has been studied based on the normalized sensitivity index defined by the following formula (21):

$$\mathrm{SI} = \frac{p}{m}\frac{\partial m}{\partial p} \quad (21)$$

where m is the methane production (m^3/d), and p is the parameter analyzed. SI represents the variation in m resulting from a 50 % increase in the parameter p. A positive value of SI means that the parameter p is positively correlated with the examined variable m, while the contrary is a negative correlation.

3.4. Validation process

This section aims to ascertain the accuracy and aptitude of the model in predicting results from defined inputs and to examine its applicability in the simulation of the AD process. For this reason, the outputs of the modified model were compared with the experimental results obtained from the two following studies extract from the literature:

- The first study, conducted by T. Thamsiriroj, concerns the modeling of mono-digestion of grass silage in a two-stage CSTR reactor using the ADM1 model [30].
- The second study, performed by Maurizio Carlini, involves the simulation of AD using a new tool called ADMS 1.0, validated by the AQUASIM software [50].

These two studies were chosen for the validation process, as they provide the bulk of the information about inputs and parameters needed to reproduce practically the same simulation conditions, which will allow testing the correctness of the results generated by the modified model.

Building on this, the effectiveness of the modified model and its ability to accurately predict the AD simulation results was assessed using the statistical measures extensively applied in the model evaluation step. The four performance factors adopted in this study are as follows: rAE (Relative Absolute Error), RMSE (Root Mean Squared Error), SI (Scatter Index), and the NES (Nash-Sutcliffe efficiency coefficient). All these statistical parameters were estimated according to the following equations (22)–(25):

$$rAE = \frac{\sum_{i=1}^{n}\left(\frac{|R_i - P_i|}{R_i}\right)}{n} \quad (22)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (R_i - P_i)^2}{n}} \tag{23}$$

$$SI = \frac{RMSE}{\overline{R}} \tag{24}$$

$$NES = 1 - \frac{\sum_{i=1}^{n} |R_i - P_i|}{\sum_{i=1}^{n} |R_i - \overline{R}|} \tag{25}$$

where n is the total number of simulated points in the reference study; R_i is the reference study value; P_i is the predicted value of the ADM1 code; and $\overline{R}$ is the mean of the reference study values.

An NES value close to 1, combined with lower rAE and RMSE values (values within an acceptable margin of error of less than 5 %) and an SI of under 10 %, all indicate a high-performing model [63].

Firstly, the conditions of operation and simulation adopted in the calibration step in the first study [30] were applied to compare the results of the biogas and methane yields illustrated in Fig. 3 (a and b) and Fig. 4 (a and b) for the modified model and the study [30] (respectively). By comparing the graphical representation of the results, it is noticeable that at the beginning of the simulation, the fluctuations in biogas yield generated by the model code tended to be slightly different from those observed in the study [30].

Secondly, using the data available in the second study [50], we compared the concentration of methane in the liquid phase and the hydrolysis components depicted in Fig. 5 (a and b) and Fig. 6 (a and b) for the ADM1 code and the study [50] (respectively). Confronting the results, it is apparent that in the last days of the simulation, the ADM1 code predicted a methane concentration value slightly higher than that registered in the study [50].

Overall, the simulation graphs (Figs. 3–6) reflect that the predicted variations of the modified model for the simulated parameters appeared very similar to the profile of the observed results reported in the references studies [30,50]. This good graphical agreement between the results is confirmed quantitatively by the lower acceptable values of the rAE and RMSE (under 5 %), an SI (less than 10 %), and NE (approaching 1) given in Table 1; all suggesting that the model exhibit a higher goodness of fit between predicted and references values.

The minimal discrepancy between the results can be explained by the default value for several parameters not specified in the reference studies. The availability of supplementary data will allow for more accurate predictions.

Generally, the validation results reveal that the model exhibits good predictive performance for the simulation of AD, especially when the modelling purpose is to forecast the main parameters relating to the energy productivity of the AD system.

It can be concluded that the modified model developed in this study can be employed in various applications, such as performing preliminary simulations to study the AD of a specified substrate or examining the effect of different parameters (for example, pH, OLR, temperature …) on the volumetric production of biogas and methane.

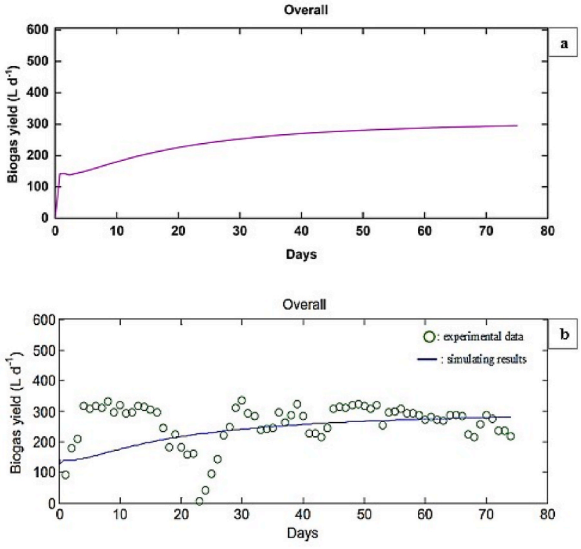

Fig. 3. Simulation results for biogas yield for the ADM1 model (a) and for the reference study (b) [30].

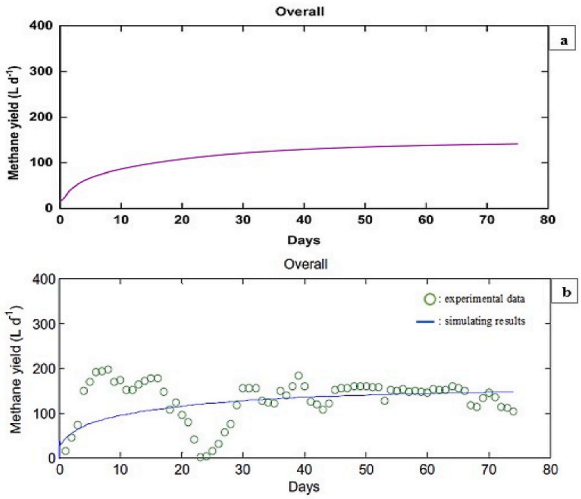

Fig. 4. Simulation results for methane yield for the ADM1 model (a) and for the reference study (b) [30].

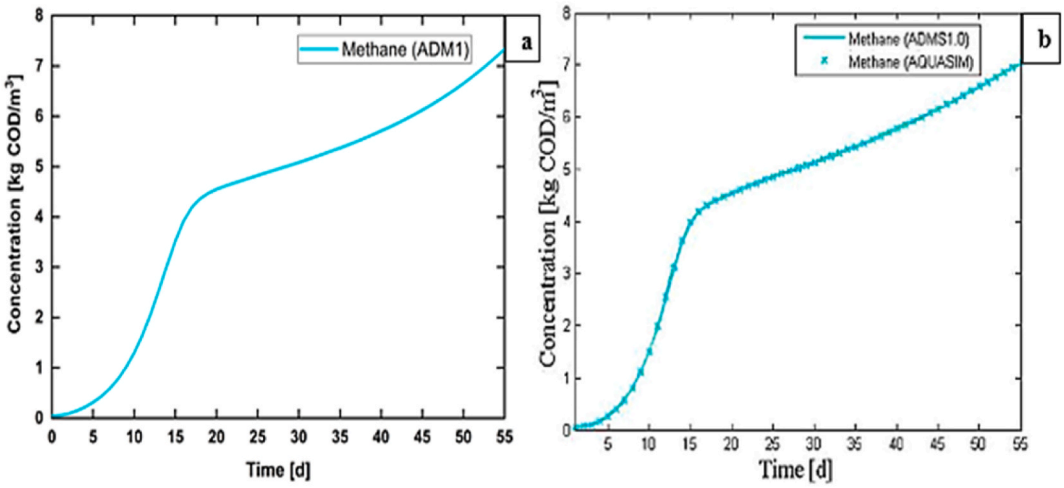

Fig. 5. Simulation results for methane concentration for the ADM1 model (a) and for the reference study (b) [50].

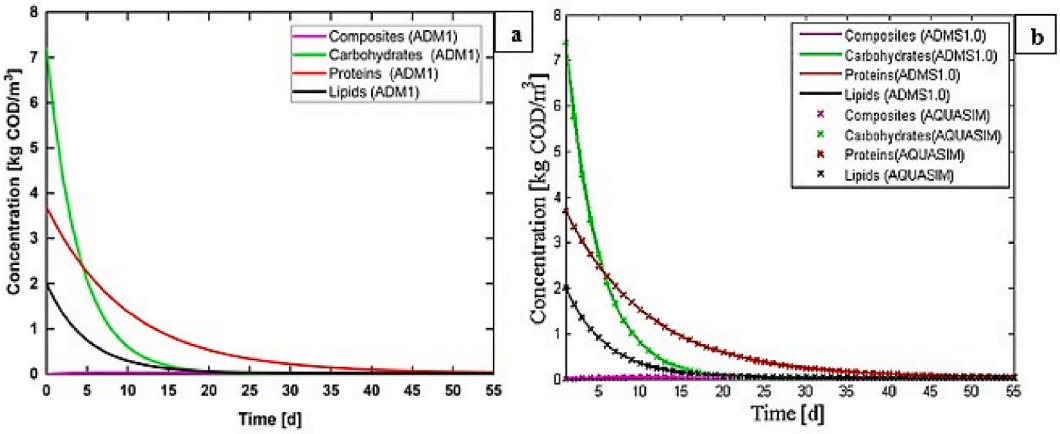

Fig. 6. Simulation results of hydrolysis for the ADM1 model (a) and for the reference study (b) [50].

Table 1
The performance metrics indicators associated to the parameters simulated by the modified model.

Parameters	rAE	RMSE	SI (%)	NE
Biogas yield ($L.d^{-1}$)	1.727	0.2965	0.2133	0.9618
Methane yield ($L.d^{-1}$)	2.11	4.002	5.3525	0.9557
Methane concentration S_{ch_4} (kg DCO/m^3)	1.4281	0.3061	8.7	0.9690
Hydrolysis (concentration of: X_c, X_{ch}, X_{pr}, and X_{li}) (kg DCO/m^3)	2.3	0.0388	1.996	0.99

4. Results and discussion

After validation of the modified model, numerical simulations were run to investigate the performances of the AD of food waste (FW) for the city of Kenitra (Morocco).

4.1. Data collection and preparation

Despite the variation in food types from one geographical region to another [64] resulting from differences in cultures and lifestyles, the basic requirements for human nutrition are similar. In this context, the Moroccan and Italian regimes are typically Mediterranean, based on consuming various products such as cereals, fruit, vegetables, and cheeses. Consequently, we can assume that the values of the main components of food waste produced by Italian and Moroccan cuisine can present a high level of similarity. Accordingly, in our study, we used data from typical food waste produced in the Italian city of Treviso collected from the study [64] (from the literature) to describe the food waste generated in the Moroccan urban area of Kenitra (lack of opportunity to conduct an experimental study). We assumed that both types of food waste have approximately identical properties in terms of physicochemical and biochemical characteristics, with insignificant differences in the values of the various parameters.

Table 2 describes the characteristics and elemental composition of the selected food waste.

- (a) No hydrogen and sulfur content values were given in the reference study [64]. Therefore, the values of H and S percentages were estimated using data from the study [65].
- (b) calculated using the following equation (26):

$$O(\%) = 100 - [C + N + H + ash] \tag{26}$$

The substrate's molecular formula was determined using food elemental analysis data. The empirical formula of the food waste was as follows: $C_{22}H_{35}O_{11}N$.

Additionally, from the characteristics and elemental composition of the selected food waste, it can be noted that the substrate:

- Contains a high proportion of VS (>70 %), which indicates the dominance of the organic matter.
- Presents a moisture content of nearly 72,5 %, which will support the activity and growth of microorganisms and facilitate the dissolution and transport of the nutrients, consequently contributing to the improvement of the decomposition of organic matter.
- Has a C/N ratio below 25 (C/N = 14,8) and a theoretical biochemical methane potential value of approximately 561 ml CH_4/g VS.

We can conclude from the information available that the type of food waste used in our study can represent a potentially suitable substrate for biogas production by anaerobic digestion.

Secondly, the ADM1 model is based on the chemical oxygen demand (COD) to characterize the different components of the organic matter and describe substrate degradation during anaerobic digestion. For this reason, the COD of the food waste was estimated by the theoretical ThCOD, which was calculated from the elemental analysis of the substrate following equation (27) [40]:

Table 2
Characteristics of food waste used in this study taken from Ref. [64].

Parameter	Value	Unit
Total Solids (TS)	27,47	% Fresh matter
Volatile Solids (VS)	23,60	% Fresh matter
Volatile Solids (VS)	86,6	%TS
Moisture Content (MC)	72,53	% Fresh matter
Carbohydrates	206	g kg^{-1} VS
Lipids	202	g kg^{-1} VS
Crude Proteins	186	g kg^{-1} VS
Total Phosphate TP (P)	3,47	g kg^{-1} TS
Nitrogen (N)	2,58	%TS
Carbon (C)	47,2	%TS
Hydrogen (H^a)	6,4	%TS
Sulfur (S^a)	0,4	%TS
Oxygen (O^b)	30,42	%TS

$$\mathrm{ThCOD} = \frac{16\,(2a + 0,5(b - 3d) - c)}{12a + b + 16c + 14d} \approx 1,6\ kg\frac{O_2}{kg\ C_{22}H_{35}O_{11}N} \tag{27}$$

4.2. Determination of the model inputs parameters

4.2.1. The input concentrations variables S and X

The values of the input concentrations for the soluble (S) and particulate (X) components of the substrate (FW) in the steady state were established using the "transformer" tool developed by Zaher [66]. This tool requires eleven input parameters estimated according to hypotheses and theoretical calculations based on the characteristics of the substrate.

Fig. 7 describes the steps required to determine the input variables for the ADM1 model.

Table 3 lists the values of the eleven parameters needed to run the "transformer".

4.2.2. Identification of the stoichiometric parameters

The value of fractions of carbohydrates $(f_{ch,xc})$, proteins $(f_{pr,xc})$, lipids $(f_{li,xc})$, particulate inert $(f_{xI,xc})$ and soluble inert $(f_{sI,xc})$ are given in Table 4. The fractions are identified on the basis of substrate composition, and have been determined by the method proposed by Koch [40], based on the following equations (28)–(30):

$$f_{ch,xc} = \frac{\%ch}{\%VS} \tag{28}$$

$$f_{pr,xc} = \frac{\%pr}{\%VS} \tag{29}$$

$$f_{li,xc} = \frac{\%li}{\%VS} \tag{30}$$

with the assumption that:

$$f_{sI,xc} = 0,1\ (by\ default); \quad f_{xI,xc} = 1 - \left(f_{ch,xc} + f_{pr,xc} + f_{li,xc} + f_{sI,xc}\right)$$

4.2.3. The biochemical parameters that need adjusting for the anaerobic digestion of food waste used in this study

Applying some kinetic parameters with their values reported in the standard version of ADM1 leads to an inexact simulation of the anaerobic digestion of food waste, resulting in inaccurate methane production results. In this context, we have focused on identifying the biochemical parameters that significantly affect methane production during the anaerobic digestion of food waste in our case. The aim is to optimize the values of these parameters to ameliorate the prediction results of the model to be approximately related to the value calculated theoretically.

a. Identification of the main parameters influencing methane production during AD of FW using a local sensitivity analysis:

To evaluate the effects of the model's input parameters on the simulated mean methane production, the parametric sensitivity analysis concerned the evaluation of the following parameters:

- The stoichiometric parameter Y that indicates biomass yield during substrate uptake.
- Four groups of biochemical parameters: the first-order disintegration and hydrolysis constants $k_{dis,inoc}; k_{dis,stub}$; $k_{hyd,ch}$; $k_{hyd,pr}$; $k_{hyd,li}$), the Monod maximum specific substrate uptake rate ($k_{m,su}$; $k_{m,fa}$; $k_{m,ac}$; $k_{m,c4}$; $k_{m,pro}$; $k_{m,h2}$; $k_{m,hSRB}$; $k_{m,aa}$), the half saturation constant for substrate degradation ($K_{S,h2}$; $K_{S,IN}$; $K_{S,aa}$; $K_{S,SO_4,hSRB}$; $K_{S,su}$; $K_{S,fa}$; $K_{S,ac}$; $K_{S,c4}$; $K_{S,pro}$) and the decay rate for substrate-degrading organisms ($k_{dec,X_{ac}}$; $k_{dec,X_{h2}}$; $k_{dec,X_{su}}$; $k_{dec,X_{aa}}$; $k_{dec,X_{c4}}$; $k_{dec,X_{pro}}$; $k_{dec,X_{hSRB}}$; $k_{dec,X_{fa}}$).
- For the remaining physicochemical parameters, for example, the gas transfer coefficient ($K_{H,gas}$), was not re-estimated in our study, as it depends on the digester configuration [67].

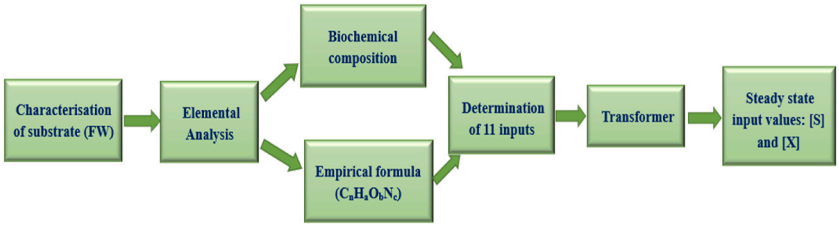

Fig. 7. The methodology followed for determining the S and X concentration input variables for the modified ADM1 model.

Table 3
The characteristics of the FW used to calculate the transformer's inputs.

Parameters	Values	Units
Particulate COD (COD_P)	430730	g m^{-3}
CODs - VFA	4395	g m^{-3}
Volatile Fatty Acids (VFA)	4395	g m^{-3}
Total Organic Carbon (TOC)	127065	gC m^{-3}
Total Organic Nitrogen (N_{org})	6304,5	g m^{-3}
Total Ammonia Nitrogen	700,5	g m^{-3}
Organic Phosphorus (TP – orthoP)	429	gP m^{-3}
Ortho – Phosphate (orthoP)	524	gP m^{-3}
Total Inorganic Carbon (TIC)	216	mole m^{-3}
Total Alkalinity (S_{cat})	25	equ m^{-3}
Fixed Solids (FS)	38700	g m^{-3}

Table 4
Stoichiometric parameters values used in the model.

Parameters	Values
$f_{ch,xc}$	0,24
$f_{pr,xc}$	0,21
$f_{li,xc}$	0,23
$f_{sI,xc}$	0,1
$f_{xI,xc}$	0,22

Fig. 9 shows the sensitivity index (SI) values calculated for the biochemical and stoichiometric parameters examined in this study.

The sensitivity index (SI) values of the yield coefficients Y against the mean methane production (Fig. 8a) showed a significant impact of acetic acid-consuming microorganisms (Y_{ac}) (SI = −0.025) and a moderate sensitivity of sugar-consuming microorganisms (Y_{su}), with an SI value of nearly - 0.018.

The sensitivity index values of the hydrolysis and disintegration parameters for the mean methane production were presented in Fig. (8e). The results revealed that the most sensitive hydrolysis parameter was the carbohydrate hydrolysis rate ($k_{hyd,ch}$), also confirmed in the study [68]. The value of the sensitivity index found in our study was almost 0.35, indicating that an increase in $k_{hyd,ch}$ implies a noticeable rise in mean methane production.

Indeed, the fact that methane production was not highly sensitive to disintegration parameters may suggest that the disintegration step is not the rate-limiting step in the AD process in our case. This result was inconsistent with the sensitivity analysis carried out in a number of studies such as [59,68], where the kinetic constant of the desintegration process was the most sensitive parameter of the ADM1 model in the case of biogas production from FW. This difference can be explained by the difference in the substrate composition used.

For the group of Monod's maximum specific absorption rate parameters, Figure (8b), showed that the highest SI was that of $k_{m,su}$ and $k_{m,aa}$ with values around 8×10^{-4}.

The $k_{m,ac}$ parameter related to methanogenesis demonstrated a moderate effect on methane production, contrasting the local sensitivity analysis reported in Refs. [59,68], where the km, ac parameter was the most sensitive among the remaining k_m rates.

The sensitivity index of the half-saturation constants against methane production was illustrated in Figure (8d). The results showed SI values around 10^{-4} for all parameters; with $K_{S,su}$ showing the highest sensitivity ($SI = -9 \times 10^{-4}$), followed by $K_{S,fa}$ ($SI = -8{,}7 \times 10^{-4}$). This may suggest that the uptake of simple sugars and long-chain fatty acids (LCFA) regulated by $K_{S,su}$ and $K_{S,fa}$ respectively have a relatively remarkable influence on reducing methane production as their values increase. The parameter $K_{S,ac}$, exhibited a relatively moderate influence ($SI = -4 \times 10^{-4}$) on methane production, while $K_{S,h2}$ showed a negligible value of SI; this was in contrast to the findings of some studies such as [59,68], which have highlighted the importance of hydrogen dynamics in the DA process.

Finally, the SI values of all decay terms were reported in Figure (8c). Among them, the decay term related to acetate-consuming bacteria $(k_{dec,X_{ac}})$ had the most significant impact on methane production (SI = 0.004), followed by the parameters $k_{dec,X_{h2}}$ and $k_{dec,X_{su}}$.

Comparing the SI values of the most sensitive biochemical parameters in each group (Fig. 9), we found that the SI of the parameters k_m, Y, and K_S were incomparable to the sensitivity index of the hydrolysis rate constant $k_{hyd,ch}$ which exhibited the highest value. This may be attributable to the high content of carbohydrates that, possibly due to their readily hydrolyzed nature, caused a rapid decomposition of the substrate, which strongly affected methane production. This suggests that these components may be closely related to methane production during AD, representing an essential factor in improving the process. Also, this may indicate the crucial role of hydrolysis in the early phases of AD, and its importance in maximizing biogas production.

Concerning the sulfate reduction process parameters ($K_{S,SO_4,hSRB}$; $k_{dec,X_{hSRB}}$) showed very low sensitivity to methane production. This can be explained by the low concentration of sulfate in the substrate associated with a low ratio (SO_4^{2-}/COD) and their contribution to

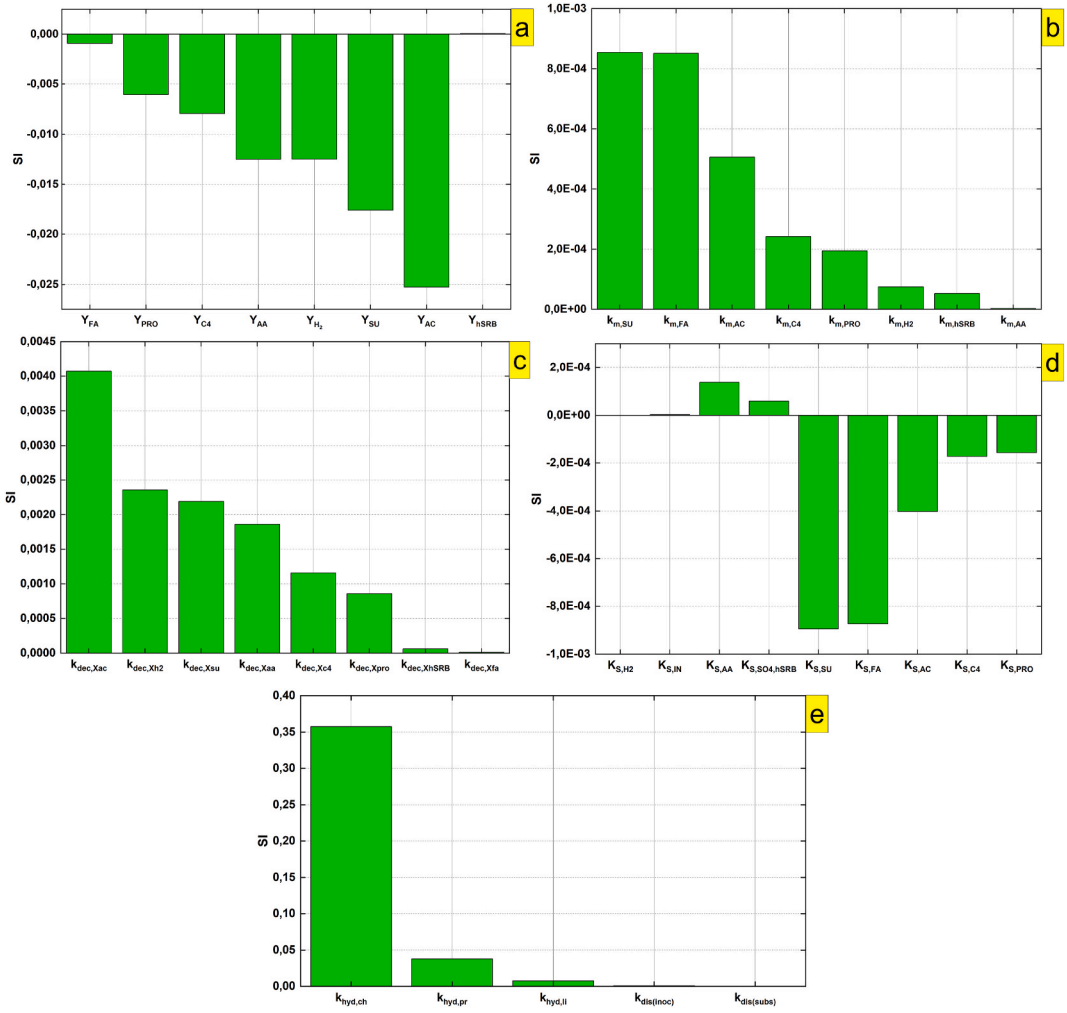

Fig. 8. Sensitivity index calculated for different model parameters referred to the mean produced methane.

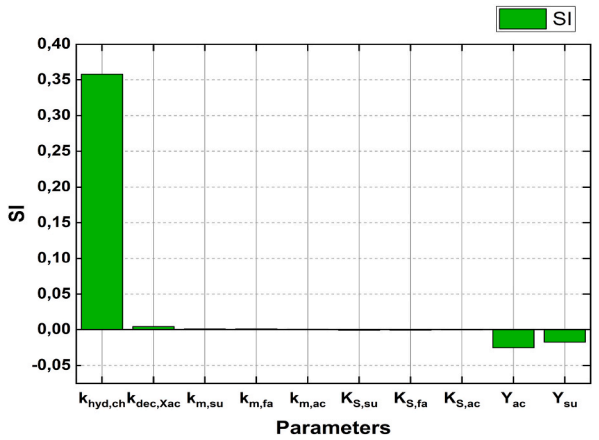

Fig. 9. Sensitivity index calculated for the most sensitive parameters of each group, for the mean methane production.

the attenuation of the activity of hSRB bacteria during AD.

The difference found in some sensitivity analysis results presented in this study compared to the literature, may be due to the different structure of the model adopted and the input data values used. Generally, the sensitivity of model parameters can change as a function of the substrate composition and its type, operational conditions, initial conditions, and also input concentrations of soluble and particulate variables in the steady state.

Consequently, the sensitivity analysis presented in this study is only a representation of a possible result that helps to offer a general overview of the biochemical parameters that can affect the model when using FW as a substrate.

b. Estimation of the sensitive parameters:

To enhance the forecasting quality of the modified model simulation results, the most sensitive parameters, determined by the sensitivity analysis ($k_{hyd,ch}$; $k_{dec,X_{ac}}$; $k_{m,su}$; $k_{m,fa}$; $k_{m,ac}$; $K_{S,fa}$; $K_{S,su}$; $K_{S,ac}$; Y_{ac}; Y_{su}) were selected for adjustment to achieve better plot quality and to obtain results close to the theoretically calculated values.

Otherwise, the theoretical maximum methane production and methane content in biogas for the FW treated in our study (calculated from the theoretical BMP) were used to calibrate the model by fitting the theoretical data to the simulated data.

The estimation of parameter values was performed with the aim of minimizing the error between the theoretical value and the model prediction (maximum value of methane production in the steady state), which was less than 5 %; reflecting the ability of the modified model to generate reasonably accurate predictions.

This approach was adopted due to the absence of an experimental study, often employed to estimate and optimize sensitive parameters using real measured methane production data.

After the calibration and validation processes, the modified model was applied in an exploratory analysis of the AD of the FW used in this study.

4.3. Performance simulation of the AD process of FW

The aim of this section is to simulate the various parameters identified as fundamental in the literature for evaluating the performance of the AD process and determining its stability. The simulation time was set to 90 days (applying a hydraulic retention time of 30 days), with an OLR of 1,652 kgVS/m3/d, in mesophilic conditions (35 °C). Steady-state conditions were assumed to be reached after approximately 80 days of operation, corresponding to the period when the simulated yields and parameters start fluctuating slightly (practically stable evolution).

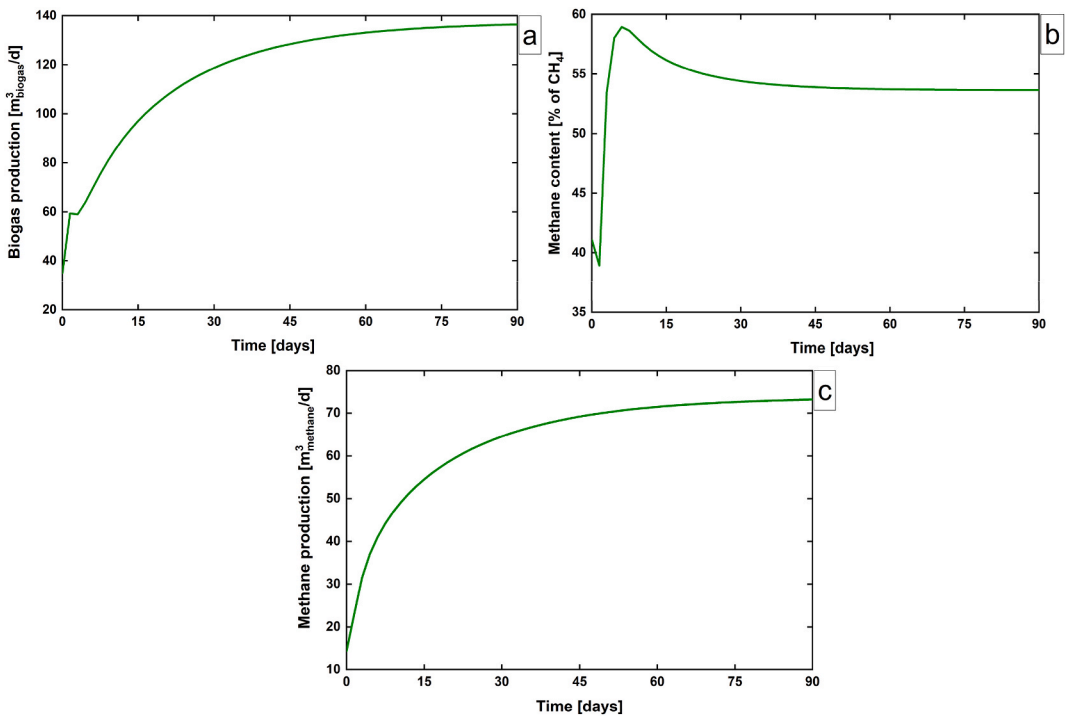

Fig. 10. (a) biogas production; (b) the quality of biogas; (c) methane production.

4.3.1. The estimation of the energetic productiveness of AD

Simulation results for daily biogas and methane production are presented in Figures (10a) and (10.c) (respectively). During the first HRT of operation, the methane production rate increases rapidly (log evolution) because the nourishment is not limited in this phase; i.e., the substrate is available and highly degraded by the microbial community that grows fast. For the rest of the simulation, methane production gradually continues increasing until it reaches the stabilization phase represented by the production curve, which tends to form a plateau. Throughout this stationary phase, the microorganisms compete for the substrate, which is all but exhausted, and the microbial reproduction rate tends to be stable. The methane production rate attained a maximum value of almost 73,21 m^3/d on day 90 (Fig. (10c)); the predicted production is less than 2,15 % of the maximum theoretical production value calculated from the theoretical BMP.

The biogas production rate is represented in Figure (11a). The production rate increases progressively during the simulation until it is approximately stable (plateau). The maximum value achieved was around 136,47 m^3/d (on day 90), which corresponds to a methane content of roughly 53,64 % (Fig. (10b)), representing more than 2,3 % of the maximum methane percentage estimated theoretically from Buswell's equation.

Additionally, other indicators are employed to evaluate energy performance, notably the BPR, SBP, MPR, and SMP.

The BPR and MPR refer to the daily production of biogas and methane per reactor volume correspondingly. Both are used in determining the efficiency of the AD process.

The SBP and SMP represent energy yields linked to the biodegradability of the feedstock and its potential in terms of energy content [69]. Both parameters are adopted in determining the biological efficiency of substrate conversion into methane and biogas [20].

The energy yields of biogas and methane are plotted in Figs. 12 and 13, respectively. The highest values reached by the SBP and the SMP during the simulation were 0,8 $m^3_{biogas}/kgVS$ (Fig. 11b) and 0,43 $m^3_{methane}/kgVS$ (Fig. 11b) (on day 90). The highest value registered by the SMP indicated that the AD process recovered almost 74,1 % of the maximum methane potential of the substrate (Table 5). The maximal values recorded for the BPR and the MPR throughout the simulation were 1,3 $m^3_{biogas}/m^3_{V_D}/d$ (Fig. 11a) and 0,7 $m^3_{methane}/m^3_{V_D}/d$ (Fig. 12a), respectively.

Based on all the simulations of the energetic parameters described previously, the results indicate a satisfactory productivity of the biogas produced by the process of AD of the FW.

4.3.2. The verification of the stability of the AD process of FW

The daily levels of the operational pH are crucial to the stability of the AD process, as they significantly affect both microbial activity and growth [51,70]. Typically, the desired pH range for the AD process is between 6,8 and 7,2 [71]. Figure (13a) shows the pH profile. As can be seen, the pH did not substantially change during the simulation, and it fluctuates very slightly around the value of 7, 16. The predicted pH values are in the range that provides a suitable environment for maintaining the high activity of methanogens [72], contributing to the efficiency of the AD process.

The changes in pH values during anaerobic digestion depend mainly on the buffer capacity of the system, which is a fundamental parameter that indicates the ability of the process to resist the falls in pH [46] caused by the accumulation of VFAs and organic overload. Alternatively, alkalinity protects the system against acidification by neutralizing the acids produced during the AD process. Figure (13b) shows the buffering capacity for the simulated process. Over the time of the simulation, alkalinity progressively increased until it began to stabilize at stable conditions. In this period, the system exhibited high alkalinity, reaching a value of almost 7 $gCaCO_3$/L. Generally, alkalinity should be above 1 $gCaCO_3$/L, and preferably between 1,5 $gCaCO_3$/L and 5 $gCaCO_3$/L [73] for the process operating under a stable state; however, higher values can be achieved in the case of AD of FW.

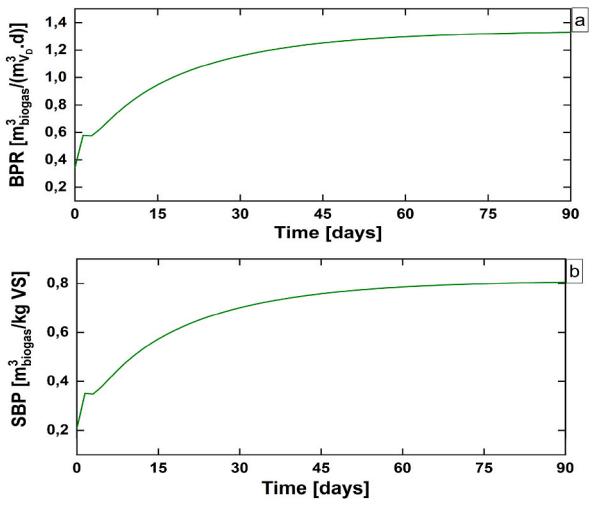

Fig. 11. Biogas energy yields; (a) the biogas production rate (b); the specific biogas production.

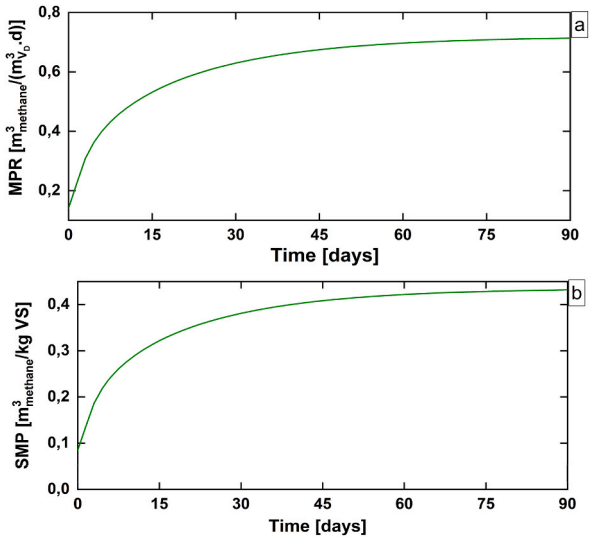

Fig. 12. Methane energy yields; (a) the methane production rate; (b) the specific methane production.

An additional factor requiring regular monitoring during the AD is the concentration of VFAs, considered a principal parameter contributing to the evaluation of the stability of the process [38], providing information that could signal the existence of instabilities inside the AD system. The VFAs are intermediates in the elaboration of methane, and they contribute to the improvement of the conversion efficiency of the substrate. However, at concentrations exceeding 800 mg/L, VFAs become components that have an inhibitory effect on the growth of methanogens [70,74].The variations in VFAs production are illustrated in Figure (13c). In the first days of the simulation, the concentration of VFAs increased significantly, rising to a value of around 111 mg/L. In the meantime, pH tended to decrease drastically. That could be related to the characteristics of the food waste, and it may suggest that these first days can represent the adaptation phase of the microorganisms to the anaerobic environmental conditions. Subsequently, the concentration of VFAs started gradually decreasing until it reached a value of 71,5 mg/L under the equilibrium conditions. This reduction results probably from the conversion of VFAs into methane via the acetoclastic methanogenic microorganisms. The variations of VFAs during the simulation are correlated positively with methane production (figure (13c)); they demonstrate the efficiency of the process in the degradation of the available organic matter. That implies that the VFAs production reactions by the acidogenesis and the acetogenesis are in balance with the VFA consumption reactions by acetoclastic methanogenesis.

An additional verification of the stability of the AD process is the determination of the concentration of total ammonia nitrogen (TAN) and ammonia (FAN). The levels of these two components are critical during the process, as elevated quantities act as inhibitors, particularly FAN, considered to be the toxic substance that strongly inhibits acetoclastic methanogenesis activity [75]. In the mesophile conditions, when the concentration of TAN is around 3000 mg/L, and the FAN exceeds 100 mg/L [76], the process could be inhibited, which may lead to the limitation or interruption of methane production. The profiles of TAN and FAN concentrations were simulated and plotted in figures (13d) and (13.e). Throughout the simulation, the concentration of TAN and FAN increased gradually until reaching their highest values of approximately 2680 mg/L and 40 mg/L (respectively) under stable conditions. The levels of TAN and FAN registered during the simulation are under the limits and do not present any inhibition risk. Instead, the values benefit the process; they contribute to the nutrients required for microbial growth and pH stability and participate in the alkalinity production and the neutralization of acids [75,77].

In addition, as stated in the literature, another way of verifying the stability of the process inside the digester is to evaluate the evolution of the stability indicators, which include the TVFAs/alkalinity ratio and the ACN index.

The TVFAs/alkalinity parameter expresses the ratio between the volatile fatty acids and the system's buffering capacity (alkalinity). It is an indicator of early failure signs of the AD process [78]. A TVFAs/alkalinity value lower than one indicates that the process is stable and operating normally; in contrast, a value higher than one shows the existence of perturbations and consequently the instability of the process [31]. The ratio of TVFAs/alkalinity over the entire simulation period is shown in Figure (14a). The plot shows that during the first days of the simulation, the ratio attains its maximum value of approximately 1,0 (the value may be slightly higher than 1 for bio-waste [31]); subsequently, the ratio starts to decrease gradually until reaching a value of 0,5 in the steady-state conditions. The registered values show healthy biological activity inside the AD system, demonstrating its stability.

The second parameter employed to identify any upcoming disturbances to the internal equilibrium of the AD process is the acetate capacity number (ACN), which is the ratio between the maximum acetate utilization rate and the acetate production rate [79]. It serves to evaluate the stability of the AD system by the determination of the capacity of the acetoclastic methanogenic microorganisms to use the excessive acetate; in other words, the quantity of the acetate exceeds the steady-state production rate [80]. ACN levels lower than one under steady-state conditions indicate a system is approaching failure [80]. Figure (14b) displays the profile of the ACN index. The values of ACN detected during the steady state simulation period were higher than 1, indicating a considerable excess capacity and the stability of the AD system operation.

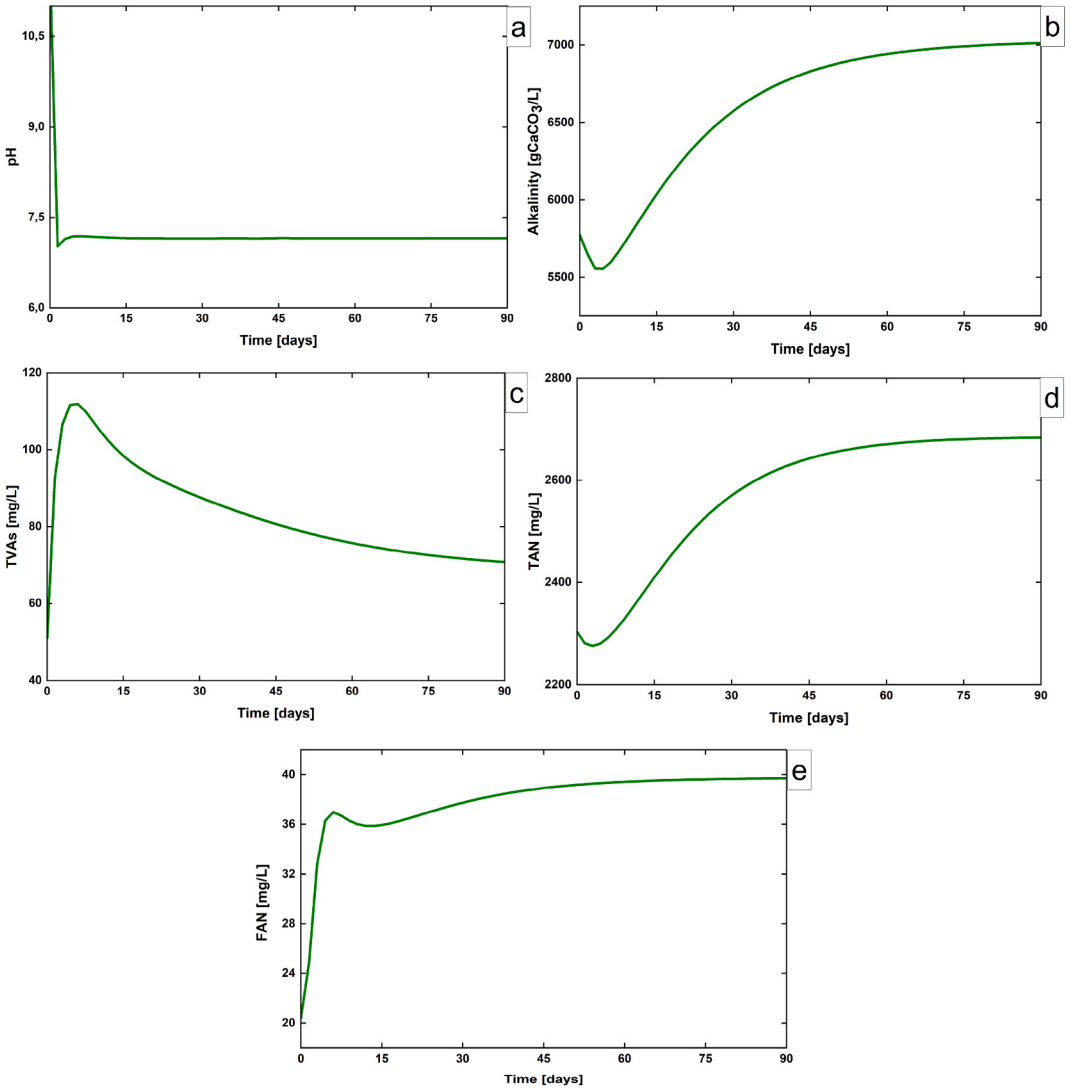

Fig. 13. Characterization of the methanogenesis process during AD of FW.

Table 5
Methane potential from FW used in this study.

	Values	Unit
Energy content of FW *(using Sheng's formula* [85]*)*	22	MJ/kgVS
The volumetric energy density of methane gas	37,78	MJ/m^3
Methane potential from FW	0,58	$m^3/kgVS$

- ***H_2S production during AD of FW:***

The AD of food waste leads to the production of hydrogen sulfide in the liquid phase, which can alter the stability of the system; in addition, its presence in the gaseous form in the biogas provokes several problems, such as corrosion of the system's equipment and the production of sulfur oxide (SOx) during combustion. For appropriate problem-solving and to ensure process stability, it is essential to evaluate H_2S production during AD and predict its evolution.

The profile of sulfate concentration variations during the simulation of AD of FW is illustrated in Fig. 15. The continuous decrease in sulfate concentration is due to its conversion by SRB bacteria into hydrogen sulfide (H_2S). The sulfate reduction was from 96 mg/L down to 4,7 mg/L (in the steady state), suggesting that perhaps the majority of sulfate was reduced during the first phase of the DA process.

The evolution of H_2S production and concentration in the biogas during the process is plotted in Figs. 16 and 17, respectively.

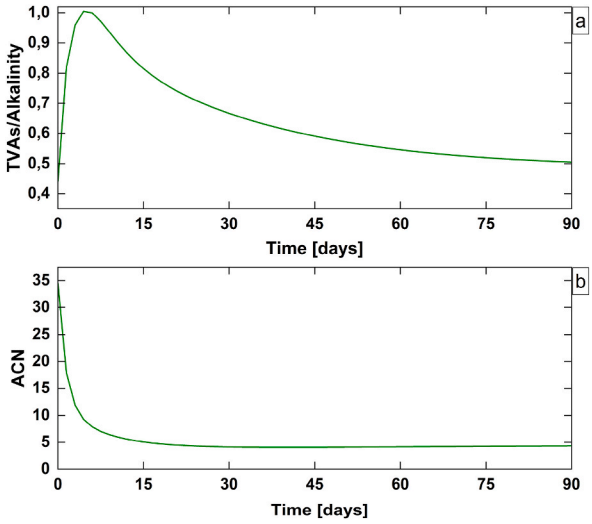

Fig. 14. Stability indicators for AD of FW.

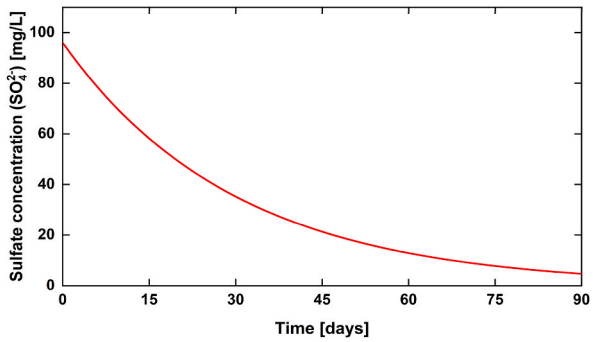

Fig. 15. The variation in sulfate concentration during AD of FW.

During the first few days of the process, the concentration and production of H_2S increase, attaining peaks of 3368 ppm and 0.20 m^3/d (representing a content of 0.3 % of the biogas), respectively.

This high production of H_2S may be explained by the sharp drop in pH (around 7), which may have encouraged the SRBs to be more dynamic, leading to the rapid degradation of most of the available sulfur into H_2S. After this phase, H_2S values tended to decline until reaching a concentration of almost 1300 ppm, corresponding to a production of 0.17 m^3/d (equivalent to 0.13 % of biogas) (Figs. 16 and 17). This reduction can be attributed to the characteristics of the substrate, which contains a low sulfur content (4 mgS/gTS), in addition to the low ratio SO_4^{2-}/COD (the theoretically calculated value was less than 0.1), which contributed to the prevention of H_2S accumulation during AD. A possible further explanation for the decrease in H_2S values could be the weakening of SRB microorganism activity due to environmental conditions favoring the activity of methanogens, such as the increase in pH levels to neutral values (around 7.16) (see Fig. 13 a).

Indeed, Fig. 18 demonstrates that despite the increase of H_2S production in the initial phase of the simulation, methane production continued to rise as hydrogen production progressed. During this period, the hydrogen produced is used as a substrate (electron donor) by both hydrogenotrophic methanogens and SRBs, but without competition-causing instabilities. This is supported by the results recorded in the steady state (Fig. 18), showing a practically stable generation of methane, accompanied by a gradual decrease in H_2S, probably due to the low conversion of the small quantities of sulfur and sulfate remaining in the DA system.

4.4. Energy and environmental advantages of AD

4.4.1. Estimating the biomethane potential generated and energy through AD

In Morocco, the technical energy potential of the waste sector was 3.1 MWh/year in 2015, including 1.8 MWh/year from organic household waste [9]. In the case of the city of Kenitra, the household waste production ratio is estimated to be almost 0.57 kg/capita/d, with a fraction of food waste (organic fraction) of nearly 83.15 % [65]. Consequently, the quantities of FW produced are about 0.47 kg/capita/d [65]. On this basis, the population of the city of Kenitra generated approximately 234 tons of FW per day, equivalent to 83, 432 tons of FW per year. These large volumes of biodegradable organic waste need to be exploited as a valuable energy resource,

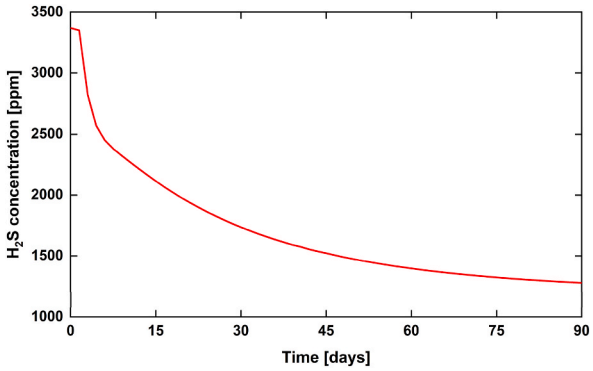

Fig. 16. Hydrogen sulfide concentration variation in biogas during AD of FW.

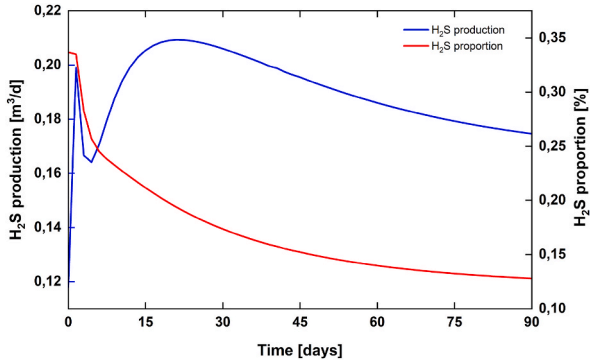

Fig. 17. Trends observed for H_2S production and its proportion in the biogas during AD of FW.

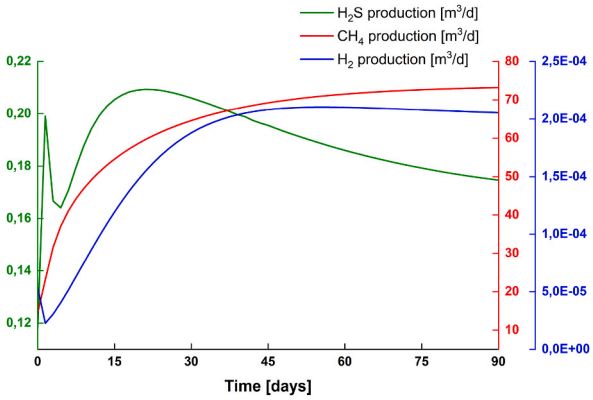

Fig. 18. Predictions of daily production of gaseous components (H_2S, CH_4 and H_2) during AD of FW.

offering the advantage of producing biogas by AD and representing an optimal solution for the waste management strategy. The ecological management of a proportion of these quantities of FW by the AD process will provide the advantage of reducing the volume of FW destined for landfills and will contribute towards sustainable development [65].

The capacity of FW to produce methane and to generate electrical and thermal energy by valorizing the biogas through cogeneration was evaluated by combining the simulation results of the ADM1 code with Matteson's estimation method [81].

Based on statistical data corresponding to the city of Kenitra, the quantity of FW generated was supposed to be entirely converted into biogas by the AD process. The theoretically estimated values for the methane volume produced and the electricity and heat energy potentials obtained by a CHP system are presented in Table 6.

From Table 6, we estimate that the treatment of food waste by AD can generate nearly 8 million m^3 of methane, having a calorific value equivalent to approximately 9.85 million tons of standard coal, calculated according to the following formula:

equivalent standard coal (tones/year) = theoretical methane volume (m^3) × 1.22 kg standard coal equivalent/m^3 methane

According to statistics from the Ministry of Energy Transition and Sustainable Development for 2022 (provisional data), the electricity demand per capita was 1154 KWh, corresponding to a daily demand of approximately 3,2 KWh per capita [82]. Consequently, the theoretical production of electricity generated from the methane produced by the AD of FW (Table 6: $E_{CHP)}$ can contribute to the satisfaction of almost 8 % of the annual electricity demand of the city of Kenitra (estimated to be 586 GWh), or it can account for 2,5 % of the electrical energy produced by the thermal power station of Kenitra in 2013 for the region of Rabat-Salé-Kenitra (the production was estimated at 1770,4 GWh) [83].

4.4.2. Carbon dioxide emission reduction via AD

To investigate the environmental benefits of the AD of FW, the emission of methane from FW and the emission resulting from utilizing biogas instead of conventional sources of fuel to produce electricity are estimated and compared.

a. Minimization of CO_2 emission by methane production:

In the majority of cases, FW is sent to landfill sites. The biodegradation of this quantity of organic matter exacerbates the climate change crisis by releasing methane. According to the standards established by the Intergovernmental Panel on Climate Change (IPCC), methane is considered a harmful greenhouse gas 21 times more potent than carbon dioxide [84]. From the annual volumetric production of methane (Table 6), it is estimated that almost 5737 tons of methane are emitted into the environment, equivalent to approximately 120477 tons of carbon dioxide. This amount of CO_2 can be reduced by AD of FW, which allows the capture of methane and its exploitation as a polyvalent source useable in a wide application range.

b. Minimization of CO_2 emission by using biogas to generate electricity:

Using an electrical conventional system (operating with standard coal) to obtain the electrical capacity in Table 6 ($E_{CHP} = 45$ GWh) can cause the emissions of nearly 42569.5 tons of CO_2 (using an emissions factor equal to 0.95 kgCO_2/KWh). While, the combustion of biogas for generating the same quantity of electricity can release almost 26886 tons of CO_2 (the value of the emission factor equals to 0,6 kg CO_2/KWh, which was estimated theoretically following the calculation method used in the study [85]), leading to a percentage saving of CO_2 of about 37 % (15683.5 tons of CO_2).

The simulation results obtained in this section, indicate that the FW can have considerable biomethane production potential under conditions favoring the stability of the process, and can be a promising source for producing bioenergy. Recycling FW by AD can be a sustainable solution for attenuating CO_2 emissions and reducing the consumption of fossil fuels through their substitution with biogas, characterized by a low carbon footprint. Integrating this approach into the national energy policy can play a significant role in the growth of the renewable energy sector.

5. Conclusion

This study has successfully developed and validated a new dynamic mathematical model tailored to simulate and forecast biogas production within the anaerobic digestion (AD) process. The AD process, recognized for its dual benefits of organic waste treatment and bioenergy production, presents significant challenges due to its inherent complexity and sensitivity to various operational conditions. By addressing these challenges, the proposed model offers a more detailed and accurate representation of the biochemical and physico-chemical processes that govern AD. The model distinguishes itself by including a thorough biochemical framework with extra information on the physicochemical processes.

The detailed local sensitivity analysis showed the necessity of selecting the correct parameters to improve the quality of the results and optimize methane production.

The model's accuracy was carefully tested using a variety of statistical indicators: the rAE and RMSE were both kept under 5 %, the SI was less than 10 % and the NES was near unity. These results confirmed the model's strong prediction accuracy when compared to other models in the literature, indicating that the model is successful at capturing the unpredictability of the biogas generation process.

The study's findings have important implications for both research and practice. For academics, the detailed model is a powerful tool for investigating the underlying mechanics of AD processes, providing insights that can help drive future advances in biogas production technology. For practitioners, the model is a helpful tool for designing, monitoring, and optimizing AD systems, resulting in steady and efficient biogas generation. This concept offers a significant step forward in terms of sustainable resource energy recovery. It serves the larger aims of waste-to-energy programs by allowing for more accurate forecasts and better control of AD processes, as

Table 6
Estimation of energy generation potential of FW valorized by AD.

	Values	Unit
Annual production of FW	87235	tones FW/year
Annual production of TS	23963	tones TS/year
Theoretical methane volume	8.08	10^6 m^3/year
Annual total heating energy from AD (H_{AD})	293.3	10^6 MJ/year
Annual CHP power generation (E_{CHP})	45	GWh/year
Annual CHP heat energy (H_{CHP})	117000	GJ/year

well as contributing to lowering waste management techniques' environmental imprint. The ability to forecast and optimize biogas production also aligns with the growing emphasis on renewable energy sources and the circular economy.

Future work could focus on further refining the model to incorporate additional variables and conditions, such as varying types of organic waste and different AD operational scales. In summary, the developed model stands as a significant contribution to the field of anaerobic digestion, offering a detailed and reliable framework for advancing biogas production technologies. Its successful validation and application underscore its potential to drive improvements in AD system performance, contributing to the sustainable and efficient recovery of energy from organic waste. This study not only addresses the current challenges in AD modeling but also paves the way for future innovations in sustainable resource management.

Data availability

Data will be made available on request.

CRediT authorship contribution statement

Miriam Mihi: Writing – review & editing, Writing – original draft, Software, Resources, Methodology, Investigation, Formal analysis, Conceptualization. **Badr Ouhammou:** Conceptualization, Methodology, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **Mohammed Aggour:** Visualization, Validation, Supervision. **Brahim Daouchi:** Supervision. **Soufyane Naaim:** Resources. **El Mahdi El Mers:** Resources. **Tarik Kousksou:** Supervision, Validation, Visualization.

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.

Appendix A

- **Structure of the modified ADM1 model:**

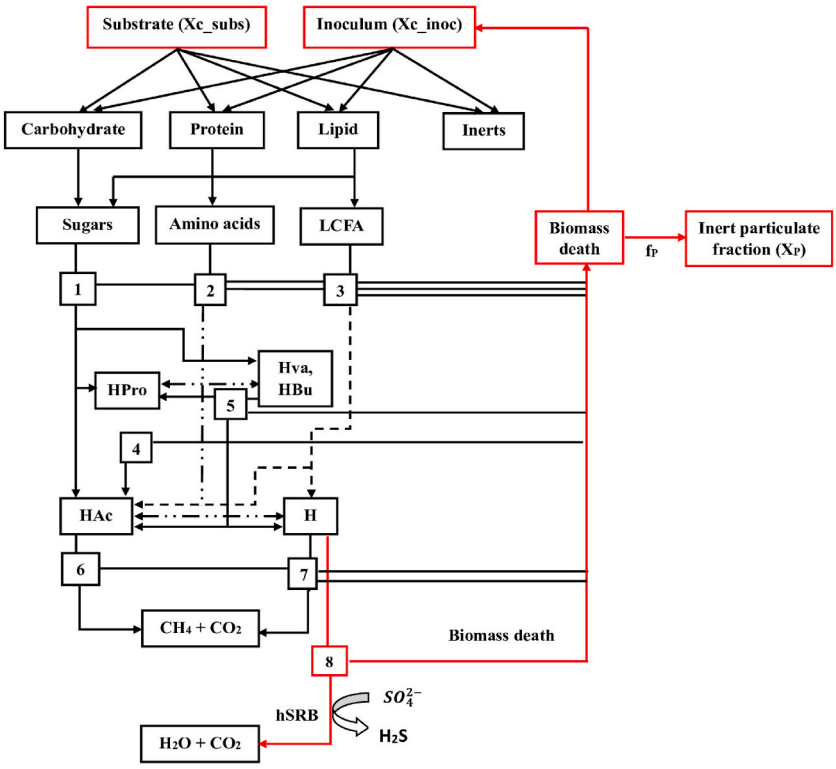

Fig. 1. The structure of the modified ADM1 model.

- **Petersen Matrix:**

Table 1
Gujer matrix of modified mathematical model equations.

Component i		8	8.a	10	11	12	12.a	13	13.a	14	15	16	24	24.a	25	Rate ρ_j (kg.DCO.m^{-3}. d^{-1})
j	Process	S_{h2}	S_{IS}	S_{IC}	S_{IN}	S_I	S_{SO4}	X_{C_inoc}	X_{C_sub}	X_{ch}	X_{pr}	X_{li}	X_I	X_{hSRB}	X_P	
1-1	Disintegration of inoculum					$f_{sI,\ xc\_inoc}$		-1		$f_{ch,\ xc\_inoc}$	$f_{pr,\ xc\_inoc}$	$f_{li,\ xc\_inoc}$	$f_{xI,\ xc\_inoc}$		$f_{xp,\ xc\_inoc}$	$k_{dis,inoc} \times a^* \times X_{C_{inoc}}$
1-2	Disintegration of substrate					$f_{sI,\ xc\_sub}$			-1	$f_{ch,\ xc\_sub}$	$f_{pr,\ xc\_sub}$	$f_{li,\ xc\_sub}$	$f_{xI,\ xc\_sub}$		$f_{xp,\ xc\_sub}$	$k_{dis,sub} \times a^* \times X_{C_{sub}}$
12-a	Uptake of hydrogen by hSRB	-1	$1 - Y_{so4}$	$-Y_{so4} * C_{bac}$	$-Y_{so4} * N_{bac}$		$\frac{(1-Y_{so4})}{64}$							Y_{SO4}		$\rho_{uptake,hSRB}$
13	Decay of X_{su}							1							f_p	$k_{dec,Xsu} \times X_{su}$
14	Decay of X_{aa}							1							f_p	$k_{dec,Xaa} \times X_{aa}$
15	Decay of X_{fa}							1							f_p	$k_{dec,Xfa} \times X_{fa}$
16	Decay of X_{c4}							1							f_p	$k_{dec,Xc4} \times X_{c4}$
17	Decay of X_{pro}							1							f_p	$k_{dec,Xpro} \times X_{pro}$
18	Decay of X_{ac}							1							f_p	$k_{dec,Xac} \times X_{ac}$
19	Decay of X_{h2}							1							f_p	$k_{dec,Xh2} \times X_{h2}$
19-a	Decay of X_{hSRB}							1						-1	f_p	$k_{dec,XhSRB} \times X_{hSRB}$
		Hydrogen gas (kg.DCO.m^{-3})	Sulfides (kg.DCO.m^{-3})	Inorganic carbon (kg.DCO.m^{-3})	Inorganic nitrogen (kg.DCO.m^{-3})	Soluble inerts (kg.DCO.m^{-3})	Sulfates (M)	Composite for inoculum (kg.DCO.m^{-3})	Composite for substrate (kg.DCO.m^{-3})	Carbohydrates (kg.DCO.m^{-3})	Proteins (kg.DCO.m^{-3})	Lipids (kg.DCO.m^{-3})	Particulate inert (kg.DCO.m^{-3})	Sulfate reducers (kg.DCO.m^{-3})	Particulate inert from biomass decay (kg.DCO.m^{-3})	

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