Contents list available at IJRED website

International Journal of Renewable Energy Development

Journal homepage: https://ijred.undip.ac.id

Research Article

Modification and extension of the anaerobic model N°2 (AM2) for the simulation of anaerobic digestion of municipal solid waste

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Abstract. Anaerobic digestion is a complex process whose understanding, optimization, and development require mathematical modeling to simulate digesters' operation under various conditions. Consequently, the present work focuses on developing a new and improved model called "AM2P" derived from the AM2 model. This new model incorporates surface-based kinetics (SBK) into the overall simulation process to transform the system into three stages: hydrolysis, acidogenesis, and methanogenesis. Experimental data from our previous work were used to identify the AM2 and AM2P models' parameters. Simulations showed that the AM2P model satisfactorily represented the effect of the hydrolysis phase on the anaerobic digestion process, since simulated values for acidogenic (X_1) and methanogenic (X_2) biomass production revealed an increase in their concentration as a function of particle size reduction, with a maximum concentration of the order of 5.5 g/l for X1 and 0.8 g/l for X_2 recorded for the case of the smallest particle size of 0.5 cm, thus accurately representing the effect of substrate particle disintegration on biomass production dynamics and enabling the process of anaerobic digestion to be qualitatively reproduced. The AM2P model also provided a more accurate response, with less deviation from the experimental data; this was the case for the evolution of methane production, where the coefficient of determination (R^2) was higher than 0.8, and the root-mean-square error (RMSE) was less than 0.02.

Keywords: anaerobic digestion; AM2 model; surface based kinetics; mathematical modeling; municipal solid waste

Received: 2nd March 2023; Revised: 24th July 2023; Accepted: 15th August 2023; Available online: 22nd August 2023

1. Introduction

Anaerobic digestion is a biochemical process that occurs without oxygen, in which microorganisms break down biodegradable organic matter to produce biogas and digestate, which is a nutrient-rich effluent. Anaerobic digestion can improve municipal solid waste management by reducing waste volume and, therefore, landfill needs, and by producing biogas that can be used as renewable energy, contributing to the conservation of natural resources and reducing greenhouse gas emissions.

Nevertheless, anaerobic digestion technology has yet to be fully mastered, and this process remains under-exploited. Mathematical modeling will allow us to understand the operation of this process and predict the performance of anaerobic digesters under different conditions. These models include mathematical equations that describe the dynamics of the microorganisms, substrates, and products of the anaerobic fermentation process; examples of mathematical models include the ADM1 model and the AM2.

Anaerobic Digestion Model No. 01 (ADM1) was created by a working group of the International Water Association in 2002. This model was designed to simulate the biochemical processes involved in anaerobic digestion. ADM1 comprises 19 different biochemical processes, each playing a specific role in anaerobic digestion. These processes include the five main steps of anaerobic digestion. The first is the disintegration step, where organic matter is broken down into smaller particles by mechanical or biological forces. This is followed by hydrolysis, in which complex polymers are broken down into simpler molecules through enzymes; then acidogenesis, where simpler molecules are converted into volatile fatty acids, alcohols, and similar compounds. The next step is acetogenesis, where the volatile fatty acids produced earlier are converted into acetate, hydrogen, and carbon dioxide. Finally, the last step is methanogenesis, where the acetates and hydrogen are converted to methane and carbon dioxide by specific methanogenic bacteria. (Li *et al*, 2019 ; Wang *et al*, 2018 ; Rozzi *et al*. 2002)

ADM1 has been extensively studied and validated by various research on anaerobic digestion. Studies such as those conducted by Batstone *et al.* in 2002 and 2003, Fezzani *et al.* in 2008, Pessoa, R.W.S *et al.* in 2019, and Sun *et al.* in 2021 have helped to improve and validate the model.

However, to use the ADM1 model, it is necessary to define 80 parameters, which makes the model quite complex to implement. These parameters include kinetic constants, mass transfer coefficients, inhibition factors, initial concentrations, and other variables that describe the characteristics of the

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https://doi.org/10.14710/ijred.2023.52798
ISSN: 2252-4940/© 2023.The Author(s). Published by CBIORE

anaerobic digestion system under study, making the model very demanding regarding input data and calibration. (Atallah *et al*, 2014 ; Capson-Tojo *et al*, 2021).

The anaerobic model n°2 (AM2) was developed within the framework of the European project AMOCO; this model considers two stages of anaerobic digestion: acidogenesis and methanogenesis. This model is represented by four state variables, with eight differential equations describing the different interactions at the two stages already mentioned, and has thirteen parameters to identify. Several authors have made improvements to this model, including (Benyahia *et al.*, 2013), who proposed the integration of the production and degradation of soluble microbial products (SMP), that their presences can present a risk of membrane fouling in the case of an anaerobic membrane bioreactor (AnMBR), now this improved model is known as AM2b; Hassam *et al.* 2015 added the decay/hydrolysis step and the release of ammonia nitrogen to the AM2 model, which allowed the integration of the substrate hydrolysis rate as a function of substrate concentration as well as the ammonium released during protein hydrolysis which can influence the alkalinity of the mixture, this model was named AM2HN; for Hess 2007 he proposed the addition of the effect of the evolution of the size of the biogas bubbles, this new model offered the possibility to include in the Am2 model, a more accurate representation of the gas/liquid volume transfer coefficient kLa, this model was named AM2G. (Benyahia *et al.* 2010; Zaatri *et al.* 2011; FEKIH SALEM.2013; Benyahia *et al.* 2013; Arzate *et al.* 2017).

Meanwhile, the present study presents a new and improved version of the AM2 model, called AM2P, which allows taking into account the influence of particle size on substrate hydrolysis. Thus, the improved AM2P model represents anaerobic digestion in three stages, adding the hydrolysis phase for the case of a batch substrate introduction system.

2. Materials and Methods

2.1 Experimental data

Our simulations were compared with experimental data obtained in our previous research (Hajji & Rhachi. 2013), which explored the effect of particle size on the anaerobic digestion of municipal solid waste from the Rabat region; these experiments were conducted through a batch-type digester of brand bioflo115 (figure1), having a useful volume of 10 liters, menu of a system of integrated control of all the operations of anaerobic fermentation, the digester functioned with a retention time of 21 days under a mesophilic regime maintained at a temperature of 40°C, thanks to a cooling circuit integrated into the vessel.

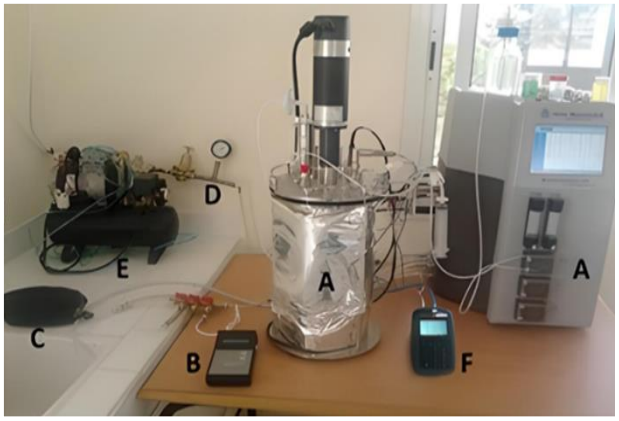

Fig. 1 Experimental digester (A) Fermenter kind BioFlo / CelliGen 115; (B) Flowmeter; (C) Gasholder; (D) Water controller for the cooling system, (E) air compressor, (F) biogas analyzer

Table 1
Physicochemical properties of municipal solid waste

Physical properties	
Density kg/m3	666.67
DM %	31.64
Humidity % (%)	68.36
OM % DM	82.3
MM % DM	17.7
Physico-chemical properties	
pH	4,86
COD mg/l	10000
TOC	45.72

In terms of measurements, the chemical oxygen demand was determined using the colorimetric method. The concentration of VFA was obtained by gas chromatography (GC). The volume of biogas was quantified using a flowmeter of the brand: Agilent ADM; as for the composition of the biogas, it was determined using a biogas analyzer of the brand GEOTECH-GA5000. The physicochemical properties of municipal solid waste are summarized in Table 1. (Hajji & Rhachi. 2022)

2.2 The Anaerobic Model N°2 (AM2)

The Anaerobic Model N°2 (AM2) is a mathematical model used to model the anaerobic digestion of organic waste. It was developed by the Institute of Agronomic Research (INRA) of Narbonne. The AM2 model is based on differential equations describing the biochemical processes involved in anaerobic digestion. The AM2 model considers anaerobic digestion a two-step process: acidogenesis and methanogenesis.

During the first step, the acidogenic microorganisms X_1 degrade the organic matter S1, representing the COD concentration, to produce volatile fatty acids (VFA) S_2. According to the reaction scheme presented below: (Rakotoniaina. 2012 ; Campos *et al.* 2022 ; Hess.2007)

$$k_1S_1 \xrightarrow{\mu_1(S_1)X_1} X_1 + K_2S_2 + K_4CO_2$$

The speed of this reaction is described by the Monod equation, which describes the growth of microorganisms as a function of the concentration of nutrients in their environment.

$$\mu(s) = \mu_{1max}\frac{S_1}{k_s+S_1} \quad (1)$$

Where μ_{1max}: represents the maximum growth rate of the acidogenic population and k_{s1} the half-saturation constant of the Monod model.

The second step is methanogenesis, in which the methanogenic microorganisms X_2 produce methane (CH_4) from the VFAs.

$$K_3S_2 \xrightarrow{\mu_2(S_2)X_2} X_2 + K_5CO_2 + K_6CH_4$$

Haldane's equation determines the speed of this reaction, which considers the inhibition by the excess of the substrate due to the

accumulation of volatile fatty acids during the methanogenesis phase.

$$\mu\,(S) = \mu_{2max}\frac{S_2}{S_2+k_{S2}+\frac{S_2{}^2}{K_{I2}}} \quad (2)$$

Where μ_{2max} is the maximum growth rate of the methanogenic population, K_{s2} is the half-saturation constant of the Haldane model, while K_{I2} is the Inhibition Constant.

The AM2 model is a system of differential equations describing substrate and product concentration dynamics over time. The acidogenic biomass concentration X_1 equation 3 is modeled using equation 5, which is based on Monod's kinetic model that describes the growth of acidogenic bacteria in the presence of a substrate.

$$\frac{dX_1}{dt} = \mu_1(S_1)X_1 \quad (3)$$

$$\Updownarrow \rightarrow \frac{dS_1}{dt} = -k_1\mu_1(S_1)X_1 \quad (4)$$

$$\mu_1(S_1) = \mu_1 \max\frac{S_1}{S_1+k_{S1}} \quad (5)$$

Equation 4 represents the change in S_1 (COD) concentration, which is directly related to the substrate concentration available to the microorganisms.

Therefore, the Monod model was used to model the consumption of organic matter and the growth of microorganisms in the bioreactor. The modeling of the methanogenic biomass concentration X_2 equation 6 is done based on the Haldane model equation 8, which predicts the reaction kinetics as a function of the substrate concentration and the substrate inhibition constant.

$$\frac{dX_2}{dt} = \mu_2(S_2)X_2 \quad (6)$$

$$\Updownarrow \rightarrow \frac{\mathrm{dS_2}}{\mathrm{dt}} = \mathrm{k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2} \quad (7)$$

$$\mu_2(\mathrm{S_2}) = \mu_2 \max\frac{\mathrm{S_2}}{\mathrm{S_2+k_{S2}+\frac{S_2{}^2}{K_{I2}}}} \quad (8)$$

Equation 7 represents the variation of the volatile fatty acid concentration S_2 using the two kinetic models, Monod and Haldane, that describe the production and consumption rates of the different types of VFA by the bacteria in the reactor.

The CO_2 volume flow rate is given by equation 9; it is a function of the total inorganic carbon concentration equation 10, the partial pressure of CO_2 equation 11, and the gas/liquid volume transfer coefficient(Rakotoniaina. 2012; Campos *et al.* 2022; Hess.2007)

$$q_C = K_{La}\,[C + S_2 - K_H P_C] \quad (9)$$

$$\frac{dC}{dt} = -qc + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2 \quad (10)$$

$$P_C = \frac{\emptyset-\sqrt{\emptyset^2-4K_H P_T(C+S_2)}}{2K_H} \quad (11)$$

$$\emptyset = C + S_2 + K_H P_T + \frac{k_6}{K_{La}}\mu_2(S_2)X_2 \quad (12)$$

Equation 13 shows the dissolved carbon dioxide concentration calculated from dissolved inorganic carbon and VFAs.

$$CO_2 = C + S_2 \quad (13)$$

The methane volume flow rate presented in equation 14 depends mainly on the growth of methanogenic bacteria, the concentration of volatile fatty acid, and the CO2 production yield.

$$q_M = k_6\mu_2(S_2)X_2 \quad (14)$$

2.3 Model development

The proposed new AM2P model was inspired by the AM2 model, based on integrating the hydrolysis phase into the overall process to transform the AM2 model into three stages. Hydrolysis is the most kinetically limiting phase of the anaerobic digestion process, which can affect the efficiency of the process. Therefore, several authors, such as hills en Nakano 1988, Hobson 1987, vaviline 1996, and Sanders *et al.* 2000, have tried to understand and simulate the behavior of the biomass during this phase by developing empirical models.

For the present work, the surface-based kinetics (SBK) model, proposed by Sanders *et al.* 2000 was chosen to simulate the hydrolysis phase; this choice was made based on our previous work on the influence of particle size on the efficiency of anaerobic digestion and which allowed us to verify and confirm the effect of the surface of the substrate particles on biogas production. (Kulkarni. 2010 ; Panico *et al.* 2014 ; Giovanni *et al.* 2011 ; Esposito *et al.* 2008 ; Dimock & Morgenroth.2006)

The SBK model represents the substrate decay kinetics based on the surface area available to the biomass according to the following expression: (Vavilin *et al.* 2008; Sanders *et al.* 2000)

$$\frac{dM(t)}{dt} = -K_{SBK} * S(t) \quad (15)$$

where: M(t) is the mass of substrate at time t, K_{SBK} is the kinetic constant of decay, S(t) is the surface available for the biomass. Assuming that the substrate consists of n spherical particles, the substrate mass can be expressed as:

$$M(t) = n * \rho * \frac{4}{3} * \pi * R(t)^3 \quad (16)$$

And

$$S(t) = n * 4 * \pi * R(t)^2 \quad (17)$$

where

$$\frac{d\left(n * \rho * \frac{4}{3} * \pi * R(t)^3\right)}{dt} = -K_{SBK} * (n * 4 * \pi * R(t)^2) \quad (18)$$

$$\frac{dR(t)^3}{dt} = -3 * \frac{K_{SBK}}{\rho} * R(t)^2 \quad (19)$$

By deriving this expression, it leads to the following result:

$$\frac{dR}{dt} = -\frac{K_{SBK}}{\rho} \quad (20)$$

Based on the assumption that the hydrolysis process continuously reduces the particle diameter, the expression for the decrease in particle size over time is as follows (Vavilin *et al.* 2008 ; Sanders *et al.* 2000):

$$R = R_0 - \frac{K_{SBK}}{\rho} * t \quad (21)$$

Where R_0: is the initial radius of the particles..

The hydrolytic biomass concentration was expressed based on the equation dM(t)/dt proportionally to a constant volume of the aqueous phase Vliq, which gives: : (Kulkarni. 2010 ; Panico *et al.* 2014 ; Esposito *et al.* 2008 ; Dimock & Morgenroth.2006)

$$\frac{dX_0}{dt} = -K_{SBK} * (n * 4 * \pi * R(t)^2) * \frac{1}{V_{liq}} \quad (22)$$

2.4 The structure of the AM2P model

The AM2P model represents an improved version of the AM2 model; it is based on the integration of the SBK model in the general process in such a way as to transform the system into three stages: hydrolysis, acidogenesis, and methanogenesis. The hydrolytic biomass concentration considers the substrate's disintegration by the effect of the particle size reduction; it is represented by the equation (25). (Kulkarni. 2010 ; Panico et al. 2014 ; Esposito et al. 2011 ; Dimock & Morgenroth.2006)

$$\frac{dR(t)}{dt} = \frac{-K_{sbk}}{\rho} \quad (23)$$

$$R(t) = R_0 - \frac{K_{sbk}}{\rho} \quad (24)$$

$$\frac{dX_0}{dx} = -K_{sbk} n 4\pi R(t)^2 \rho \frac{1}{V_{liq}} \quad (25)$$

$$\frac{dS_1}{dt} = K_{sbk} n 4\pi R(t)^2 \rho - k_1 \mu_1(S_1) X_1 \quad (26)$$

$$\frac{dX_1}{dt} = \mu_1(S_1) X_1 \quad (27)$$

$$\mu_1(S_1) = \mu_{1max} \frac{S_1}{S_1 + k_{S1}} \quad (28)$$

$$\frac{dS_2}{dt} = k_2 \mu_1(S_1) X_1 - k_3 \mu_2(S_2) X_2 \quad (29)$$

$$\frac{dX_2}{dt} = \mu_2(S_2) X_2 \quad (30)$$

$$\mu_2(S_2) = \mu_{2max} \frac{S_2}{S_2 + k_{S2} + \frac{S_2^2}{K_{I2}}} \quad (31)$$

$$\frac{dC}{dt} = -qc + k_4 \mu_1(S_1) X_1 + k_5 \mu_2(S_2) X_2 \quad (32)$$

$$q_C = K_{La} [C + S_2 - K_H P_C] \quad (33)$$

$$q_M = k_6 \mu_2(S_2) X_2 \quad (34)$$

Table 2
Initial conditions of the AM2P model

Variable	Value
S1(0) [g.L-1]	10.00
S2(0)[mmol.L-1]	1.01
X0(0)[g.L-1]	3.00
R(0)[cm]	0.5 / 1 / 1.5 / 5
X1(0)[g.L-1]	0.36
X2(0)[g.L-1]	0.23
C(0)[g.L-1]	2.94

(Zaatri *et al.* 2011 ; Houngue *et al.*2015)

2.5 Model calibration

The initial conditions used during the simulation of the AM2P model are given in Table 2.

The hydrolysis constant, relative to the KSBK surface, was identified while trying to reduce the discrepancy between the simulation results and the experimental data. (Panico *et al.* 2014; Esposito *et al.* 2008; Dimock & Morgenroth. 2006)

The substrate density was determined experimentally; the number of particles was calculated from the total mass of material and the mass of an elementary particle according to the following formula:

$$n = \frac{M_{totale}}{M_{particule}} = \frac{(X(0).V)}{\frac{4}{3}.\pi.R(0)^3.\rho} \quad (35)$$

The coefficient of determination (R2) and the root mean square error (RMSE) were used to measure the difference between the predicted and measured values to evaluate the accuracy of the predicted value. These two evaluation coefficients were explicitly applied to methane production data since methane production represents the most crucial output data, which reflects the reliability and quality of the model used. For a better fit between the measured and simulated values, the R2 value should be close to 1, and the RMSE value should be low; however, the closer the R2 value is to 0, the larger the RMSE value is, the worse the fitting effect is.

The coefficient of determination (R^2) and the root mean square error (RMSE) were calculated using equations 36 and 37:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}((y_{m,i} - y_{s,i})^2}{\sum_{i=1}^{n}((y_{m,i} - \bar{y}_{m,i})^2} \quad (36)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_{s,i} - y_{m,i})^2}{n}} \quad (37)$$

Where y_{exp} : experimental data, y_{sim} : simulated data. v_{exp} : the average of the experimental data

3. Results and Discussion

3.1 Model validation

The parameters of the new AM2P model have been identified from an experimental data set referring to our previous work and based on the most used values in the literature of the

Table 3
AM2P model calibration parameters compared with AM2 model parameter values from the literature.

Parameters	Units	AM2P model values	Most used values of the AM2 model
$\mu_{1\,max}$	1/j	0.299	0.3
K_{s1}	g/l	6,00	7.1
$\mu_{2\,max}$	1/j	0.137	0.19
K_{s2}	g/l	1.90	1.80
K_{I2}	g/l	19.20	19.20
K_1	g/g	7.50	6.00
K_2	g/g	6.99	6.99
K_3	g/g	3.70	3.80
K_4	g/g	12.61	8.62
K_5	g/g	20.00	21.00
K_6	g/g	3.80	5.99
K_H	g/L.atm	1.62	1.62
K_{la}	1/j	6.48	4.48
K_b	-	6.5 10-7	6.5 10-7
K_{sbk}	g/cm2.j	0.00096	-
P	g/cm3	0.77	-
N	-	104.64	-

(Panico *et al.* 2014 ; Esposito *et al.* 2008 ; Noykova *et al.* 2002 ; Gavala *et al.* 2003 ; Benyahia. 2012 ; Zaatri *et al.* 2011 ; Houngue *et al.* 2015 ; wen-der & chi-yuan 2007 ; Bernard *et al.* 2001 ; Hess. 2007)

parameters listed in Table 3 to obtain the best fit with the experimental results.

During anaerobic digestion, substrate particles decrease in size over time. As the anaerobic digestion process proceeds, the anaerobic microorganisms actively digest the substrate and produce enzymes that break down complex substrate molecules into smaller, more metabolizable molecules. As the microorganisms grow and multiply, their enzymatic activity continues, causing the substrate particles to break down into smaller pieces. This leads to destructuring of the substrate particles and fragmentation. (Li *et al*,2019; Cano *et al*, 2014; Xu *et al*, 2015)

Particle size reduction during anaerobic digestion was studied using the Sanders model (Equation 21), which predicts the degradation rate of organic particles in an anaerobic digester as a function of particle size. According to this model, the degradation of organic particles in an anaerobic digester depends on the total surface area of the particles, which is directly related to their initial radius. The model assumes particle radius decreases during anaerobic digestion due to particle disintegration. (Emebu *et al*, 2022)

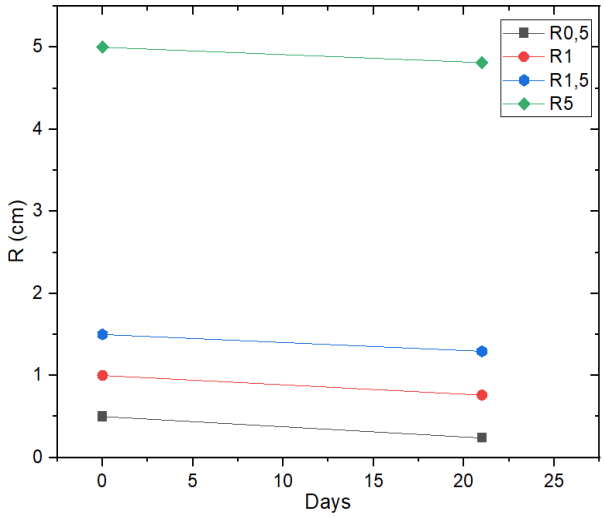

Fig. 2 Simulation of particle size reduction with different initial conditions

Figure 2 shows the model responses for particle size reduction for the four initial particle radii, 0.5, 1, 1.5, and 5 cm. The curves show that the smaller the particle size, the greater the percentage of particle size reduction, as a particle size reduction of 34% was recorded for an initial substrate radius of 0.5 cm, 17% for an initial radius of 1 cm, 11.33% for an initial radius of 1.5 cm, and 3.4% for an initial radius of 5 cm. (Emebu *et al,* 2022)This can be justified because larger particles have a smaller surface area per unit volume and are degraded less rapidly than smaller particles. These results agree with Harshad Vijay Kulkarni's work (Kulkarni., 2010). Accordingly, it can be confirmed that the model is sensitive to particle size reduction.
Biomass production in an anaerobic digester is influenced by several factors, such as substrate composition, digester operating conditions, and hydraulic retention time (HRT). Hydrolytic, acidogenic, and methanogenic biomass evolution in an anaerobic digester is a dynamic and complex process. These three types of biomass play distinct roles in the degradation of organic substrates and biogas production. The hydrolytic biomass consists of microorganisms responsible for the initial degradation of complex organic substrates into volatile fatty acids, sugars, amino acids, etc. At the beginning of the anaerobic digestion process, hydrolytic microorganisms use the available substrates to produce energy and new microorganisms. As digestion continues, the concentration of substrates decreases, and the production of hydrolytic biomass slows down. Acidogenic biomass includes microorganisms that convert hydrolyzed products (volatile fatty acids, sugars, amino acids) into simpler volatile fatty acids such as acetic acid, propionic acid, and butyric acid. These microorganisms are usually acid-forming bacteria. As anaerobic digestion progresses, the acidogenic biomass grows to efficiently convert the hydrolyzed products into volatile fatty acids. Methanogenic biomass, on the other hand, is composed of methanogenic microorganisms that use the volatile fatty acids produced by the acidogenic biomass as a substrate to produce methane (CH_4) and carbon dioxide (CO_2). Methanogens are specialized bacteria that produce biogas primarily composed of methane. At the beginning of the anaerobic digestion process, methanogenic biomass may take longer to develop than acidogenic biomass, as it requires more specific conditions and slower adaptation. (Wang *et al*, 2018; D'Silva *et al*, 2021). As the anaerobic digestion process stabilizes, the evolution of acidogenic and methanogenic biomass tends to reach an equilibrium. A proper balance between these two types of biomass is essential for efficient anaerobic digestion and optimal biogas production. (Kythreotou *et al*, 2014; Lauwers *et al*, 2013)

From the simulation results of the biomass concentration for different initial particle radii, presented in Figure 3, it was noticed that the particle size significantly influences the biomass concentration; this is because the growth of these bacteria strongly depends on access to the organic substrates present in the particles. When particle size is reduced, the specific surface area of the particles increases, allowing greater exposure of organic substrates to the bacteria. In addition, a reduction in particle size can also increase the enzymatic activity of anaerobic bacteria, as it facilitates access to organic substrates

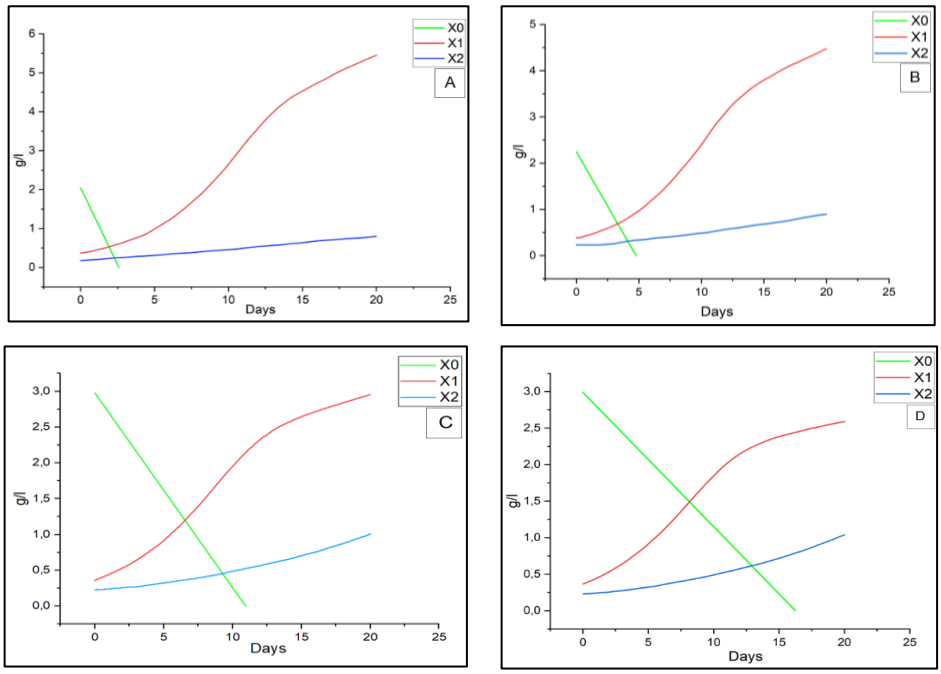

Fig. 3 Simulation of the biomass concentration X_0, X_1 and X_2 for different particle radii, A: R_0=0.5cm; B: R_0=1cm; C: R_0=1.5cm; D: R_0=5cm

and their hydrolysis into more readily available soluble products; this can lead to an increase in the rate of degradation of organic substrates and an acceleration of bacterial proliferation. Therefore, the choice of small-size particles favors the development of the two archaea involved in the anaerobic digestion process: acidogenic and methanogenic this is what has been deduced from Figure 3, where it can be noticed that the smaller the particle size, the higher the concentrations of acidogenic and methanogenic biomass. Thus, smaller particle sizes allow equilibrium to be reached more quickly because the substrate is hydrolyzed more quickly than with larger particles (Benyahia *et al*., 2013; Zaatri and Kelaiaia 2020; Bandgar *et al*, 2022). This can lead to an increase in the degradation rate of organic substrates and an acceleration of bacterial proliferation. Consequently, the choice of small-size particles favors the development of the two archaea involved in the anaerobic digestion process: acidogenic and methanogenic archaea. Figure 4 shows the variation of the simulated and measured

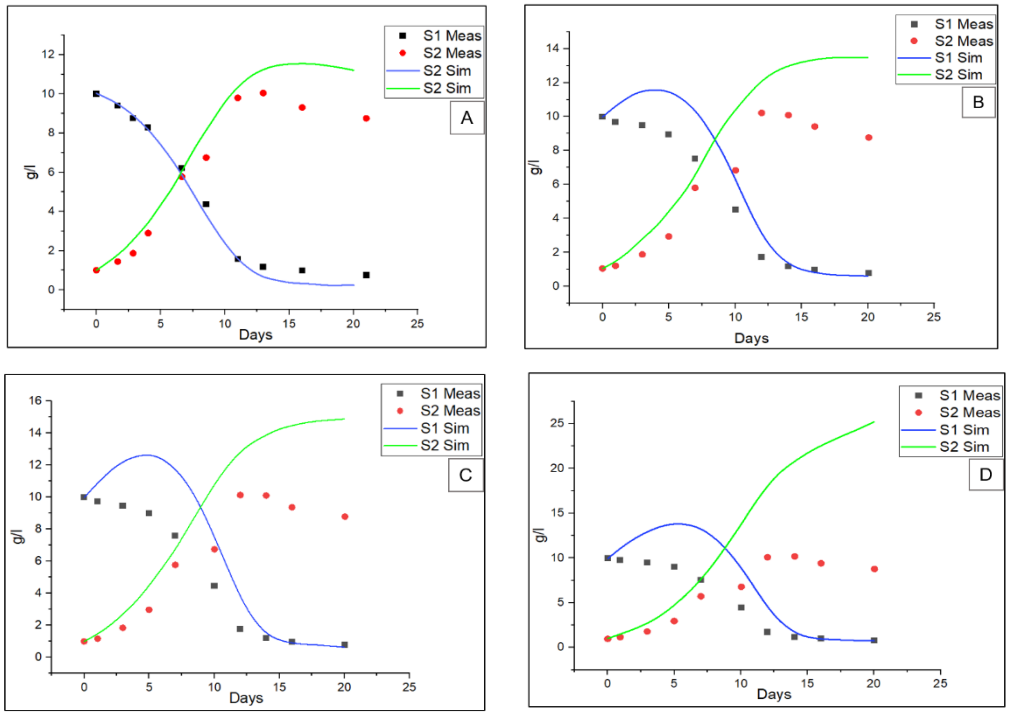

Fig.4. Measured and simulated concentrations of substrate S1 and S2 for different particle radii, A: R_0=0.5cm; B: R_0=1cm; C: R_0=1.5cm; D: R_0=5cm

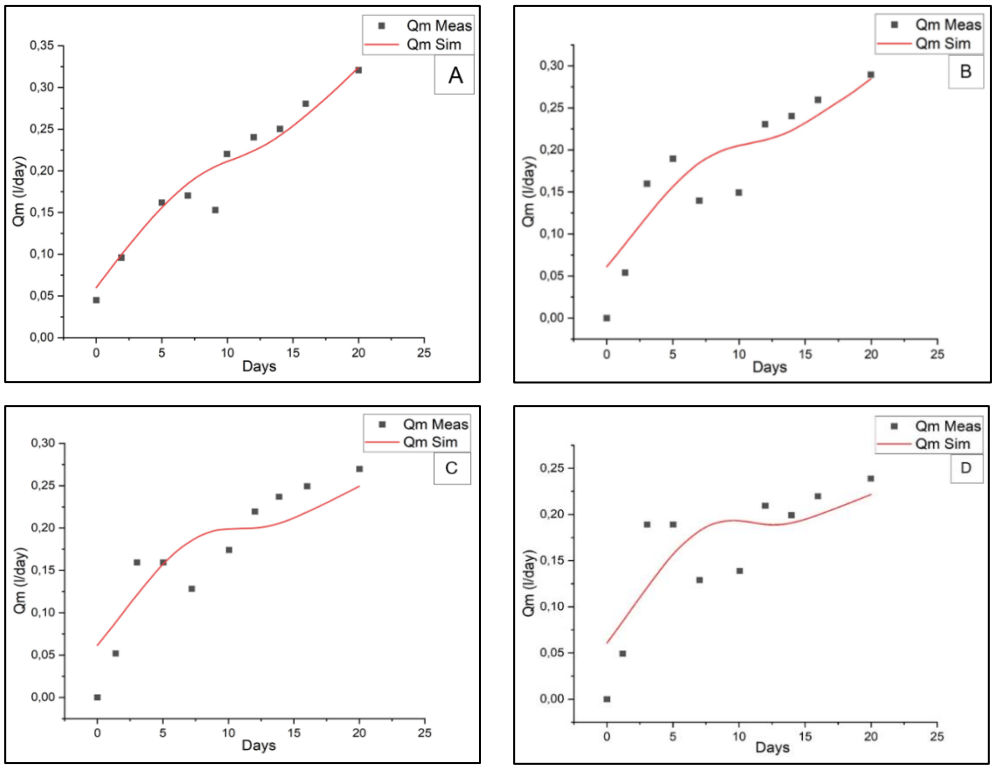

Fig.5. Measured and simulated methane production for different particle radii, A: R_0=0.5cm; B: R_0=1cm; C: R_0=1.5cm; D: R_0=5cm

concentration of S_1 (COD concentration) and S_2 (Volatile Fatty Acid concentration); it can be noticed that at the beginning of the digestion, the S_1 substrate concentration registered a slight decrease due to the release of easily degradable organic compounds such as carbohydrates and proteins. The bacteria then metabolize these compounds to produce VFAs such as acetic acid, propionic acid, and butyric acid (Benyahia *et al.* 2013; Zaatri and Kelaiaia. 2020)

As anaerobic digestion progresses, the S_1 substrate concentration decreases further as the bacteria degrade the substrate's organic compounds. At the same time, the S_2 substrate concentration increases due to the continued production of VFAs by the bacteria. However, the VFA production reaches a maximum at a certain point of the anaerobic digestion, after which the VFA concentration starts to decrease due to the continuous consumption of VFA by the bacteria to produce methane.

From these results, the simulation could reliably reproduce the dynamics of S_1 and S_2 concentrations. It was also noticed that when the particle size is reduced, the substrate is degraded more rapidly since a reduction in particle size leads to a proportional increase in the surface area available for biomass growth, thus avoiding the accumulation of substrate that can slow down anaerobic digestion.

Thus, an agreement was observed between the simulation results and the experimental data. Nevertheless, one recorded a slight difference between the two curves of the simulated and measured data, which becomes more critical with the increase of the particle size, which may be due to the modifications one made to the model structure since one adapted it to the batch system by adding the hydrolysis phase in the model.

Reducing particle size improves the accessibility of nutrients and organic substrates to methanogenic microorganisms, favoring their growth and multiplication, thus increasing methane production. Indeed, small particle size increases the specific surface area for microorganisms to adhere to and degrade organic matter, stimulating their metabolic activity and growth, as Figure 3 shows where the concentration of acidogenic and methanogenic biomass increases with particle size reduction.

All of the above was confirmed by the results in Figure 5, which compares simulation data and experimental results of methane production for different particle sizes. From the results, it was deduced that the model correctly predicted the methane production process; since the methane production increases by reducing the particle size, it was found that the more the particle size is reduced, the better the model predicts the simulation data and the gap between the simulated and measured data is reduced more, this was supported by the values of the coefficient of determination (R^2) and the root-mean-square error (RMSE), where a value of R^2 and RMSE was recorded respectively of 0. 97 and 0.01 for the case of particle size of 0.5 cm, 0.94 and 0.014 for the case of particles of 1 cm, 0.87 and 0.017 for the case of particles of 1.5 cm, as well as 0.8 and 0.02 for particles of 5 cm. From these results, it can be deduced that the model predicted the dynamics of methane production satisfactorily since the R^2 values for the different particle sizes were higher than 0.8 and with RMSE values lower than 0.02, which indicates the validity of the new AM2P model.

3.2 Model comparison of AM2P / AM2

The simulation results of S_1 and S_2 substrate concentration and methane production obtained from AM2 and AM2P models show that both models can be adapted to simulate a batch system with municipal solid waste as substrate. It was also found that the AM2P model reproduced the anaerobic digestion process better than the AM2 model, with slight differences between the experimental and simulated data, as shown in Figure 6. The AM2P model satisfactorily represented the effect

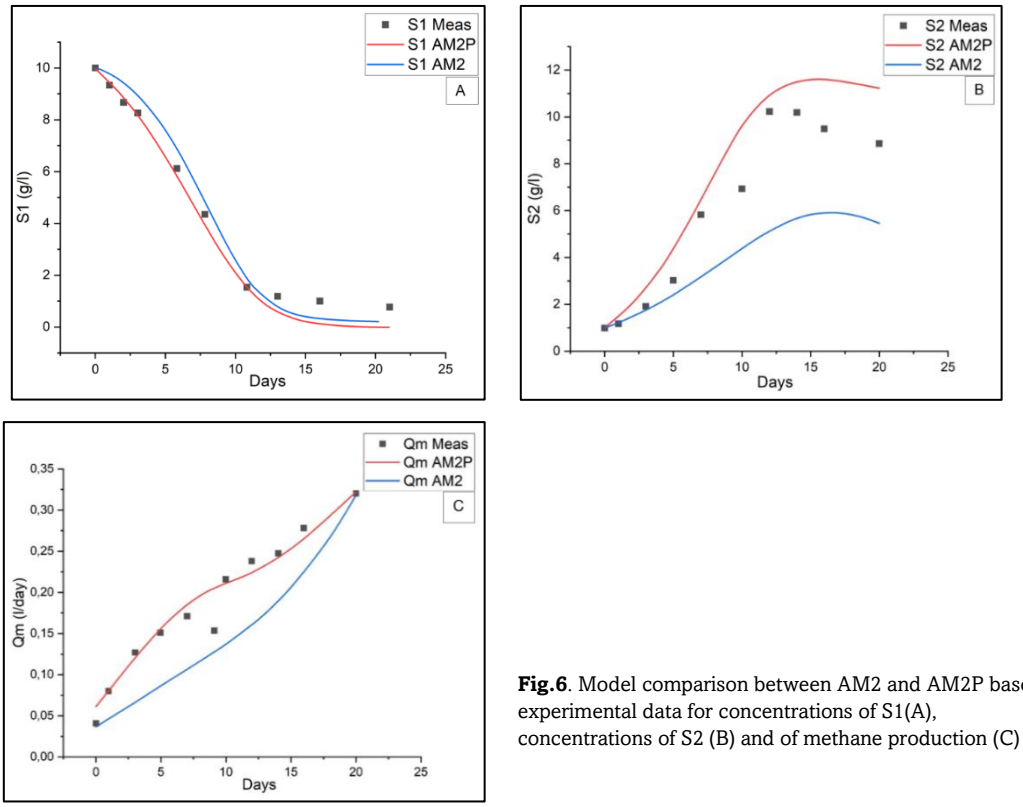

Fig.6. Model comparison between AM2 and AM2P based on experimental data for concentrations of S1(A), concentrations of S2 (B) and of methane production (C)

of the hydrolysis phase on the anaerobic digestion process, which allowed the system to perform better and therefore produce more reliable simulation results than the AM2 model; this was also supported by the values of the coefficient of determination (R2) which presented a better value of 0.97 recorded for the case of the data simulated with the AM2P model. However, the AM2 model presented an R2 value of 0.93, similar to the root-mean-square error (RMSE), which recorded a lower value of 0.01 for the case of the AM2P model than for the AM2 model, which displayed a value of 0.019. Nevertheless, the AM2 model finds its limits when changing the size of the substrate particles, which makes our new AM2P model a qualitative improvement of the AM2 model. However, the AM2 and AM2P models failed to correctly reproduce some variables, such as inorganic carbon concentration, because both models were transformed and fitted to the batch system.

4.Conclusion

As part of this work, an improved model for the anaerobic digestion of municipal solid waste called "AM2P" was developed based on the AM2 model, integrating the hydrolysis phase into the overall process to transform the AM2 model into a three-stage process. The parameters of the AM2 and AM2P models were identified based on experimental data from previous work. The simulations carried out showed that the new AM2P model was able to improve the accuracy of the simulation of the anaerobic digestion process compared to the AM2 model, reducing the deviation from the experimental data, and representing the evolution of the different archaea as well as the production of methane in a relatively reliable way, with recorded values of R2 higher than 0.8 as well as RMSE values lower than 0.02. Simulation results also revealed that the AM2 model found its limits when changing substrate particle size, making the new AM2P model a qualitative improvement on the AM2 model.

Prospects for future work include: (i) the introduction of new variables such as agitation and temperature to the AM2P model, (ii) the addition of similarity criteria concerning the dimensions of the bioreactor used (field of validity of the AM2P model in terms of digester size) to make it as complete as possible and usable by industrialists and researchers interested in the biogas field.

Nomenclature

C	Total inorganic carbon concentration g.L-1
k_1	Substrate degradation efficiency g.g-1 acidogenic biomass
k_2	VFA production efficiency g.g-1 acidogenic biomass
k_3	VFA degradation efficiency g.g-1 methanogenic biomass
k_4	CO_2 production efficiency from S_1
k_5	CO_2 production efficiency from S_2
k_6	CH_4 production efficiency from S_2
K_H	Henry's law constant g.L-1.atm-1
K_{La}	Gas/liquid volume transfer coefficient days-1
K_{I2}	Inhibition constant g.L-1
K_{S1}	Half-saturation constant of the Monod model g.L-1
K_{S2}	Half-saturation constant of the Haldane model g.L-1
P_C	Partial pressure of CO_2 Atm
P_T	Total pressure Atm
q_C	Volume flow of CO_2 L. day -1
q_M	CH_4 volume flow rate L. day -1
S_1	COD concentration in the reactor g.L-1
S_2	VFA concentration in the reactor mmol.L-1
X_0	Hydrolytic biomass concentration g.L-1
X_1	Concentration of the acidogenic population g.L-1
X_2	Methanogenic population concentration g.L-1

μ_1	Growth rate of the acidogenic population days-1
μ_{1max}	Maximum growth rate of the acidogenic populationdays-1
μ_2	Growth rate of the methanogenic population
μ_{2max}	Maximum growth rate of the methanogenic population
k_{SBK}	Surface-based hydrolysis constant

Author Contributions: A.H.: Conceptualization, methodology, formal analysis, writing—original draft, Y.L.; Resources, formal analysis, validation, M.G.; Software, validation, visualization, N.L.: Resources, project administration, validation, M.R.; Methodology, supervision, project administration. All authors have read and agreed to the published version of the manuscript.

Funding: The authors received no financial support for the research, authorship, and/or publication of this article.

Conflicts of Interest: The authors declare no conflict of interest.

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