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Analysis and Simulation of AM2 Model for Anaerobic Digesters

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Abstract. The simulation of anaerobic bioreactors of batch type for the methane production according to the AM2 mathematical model reveals a strong sensitivity of the results (variation of the concentrations of substrates, bacterial evolution and flow of methane production) with respect to the variations of the model parameters. To highlight this sensitivity, we undertook an extensive literature review that has actually shown a dispersion of the model parameters as given and estimated by different authors. This is due, probably, to the complexity of biotechnology phenomena, to the variety in the composition of the substrate and to other factors influencing the experimental conditions (pH, temperature, etc.). An "average" estimation of the model parameters based on the literature was determined and was used to simulate the operation of the bioreactors. A comparative analysis of this model is performed enabling to show the variability of the system parameters and its influence on the methane production. By fitting the shape of the simulated model to that of experimental results given by the literature, we extract some average parameter values that can be used later on to characterize bioreactor systems in more or less similar conditions.
Keyword: *Anaerobic digestion, AM2 model, Simulation of anaerobic bioreactors, Biotechnology.*

The exploitation of bioreactors by farmers to produce methane dates already from many decades. It was initially considered as a natural way to produce energy economically especially during oil crisis. Later on, it was considered also as an interesting alternative to oil energy among other renewable energies such as solar, wing, and so on. However, the process of producing renewable gas is gaining more interest since the last decade as one mean to fight against climate change by reduction of CO_2 emission.

The anaerobic digestion is a phenomenon of an extreme complexity which has opened numerous ways of research in microbial ecology, molecular biology, microbial physiology, taxonomy, energy production, biotechnology, etc.

The phenomenon in itself takes place in ecosystems of an extreme diversity such as marine sediments, extreme thermophilic or halophilic mediums, in the gastro–intestinal tract of ruminants and many other animals, soils, anaerobic digesters [ZEIKUS *et al.*, 1977; ZEHNDER *et al.*, 1980; OLIVEIRA *et al.*, 2018]. In spite of this diversity, the concept of anaerobic digestion can express itself in a relatively unitarian theory, the variants of which apply to the peculiarities of the studied mediums: competitions between microorganisms according to the mineral acceptors of present electrons [OLIVEIRA *et al.*, 2018; KRISTJANSSON *et al.*, 1982; SCHONHEIT *et al.*, 1982] according to the conditions of environment [ZEIKUS *et al.*, 1977].

From the technological viewpoint, the anaerobic digestion has a particular importance because it can constitute a renewable energy source for methane production as well as a means to reduce the pollution. To analyze the functioning of anaerobic digesters and to predict their performances, the modeling and the simulation stands as a very economic and flexible technique.

The first mathematical models of anaerobic bioreactors were proposed since the 1970s. Since then, more or less complex models according to the number of considered biochemical processes were proposed. The ADM1 model for

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Banat's Journal of Biotechnology
2020, XI(22)

"Anaerobic Digestion Model n°1 is a model which was developed by the researchers of the IWA (International Water Association) [VAVILIN *et al.*, 2000].

It is a very complete model allowing to simulate at best the anaerobic reactors. Nevertheless, this model is very complex because it describes 19 biochemical processes, 3 kinetic processes of gas–liquid transfers and 7 different bacterial populations. This model requires the adjustment of more than 80 parameters. On the other hand, the AM2 model, which was developed in 2001 by the INRIA, is a very useful one because it reconciles precision and complexity. It requires fewer parameters [Reynard *et al.*, 2007].

The simulation of anaerobic bioreactors of batch type by means of a program we have developed according to AM2 mathematical model showed a strong sensibility of the results (variation of the substrate, evolution of bacteria and methane production) with respect to the variations of the model parameters.

This depends, doubtless, in the complexity of the biotechnological phenomena, in the variety in the composition of the substratum and in the numerous factors influencing the experimental conditions (pH, Temperature, etc.).

An extensive bibliographical analysis concerning the model AM2 was made in order to determine the values of the used parameters. It allowed to consider the "average" parameters of the model with regard to the data supplied by various authors.

A simulation of the functioning of the bioreactor with these data was made followed by a comparative and critical analysis of this model, enabling to show the variability of the system parameters and its influence on the methane production.

Presentation of the AM2 model

Biological Processes of the AM2 model

The mathematical model of the anaerobic digestion (AM2) is based on two main reactions, where the substrate S_1 is degraded into a substrate S_2 by bacteria X_1 then the substrate S_2 is degraded by bacteria X_2 to supply the biogas (see Figure 1).

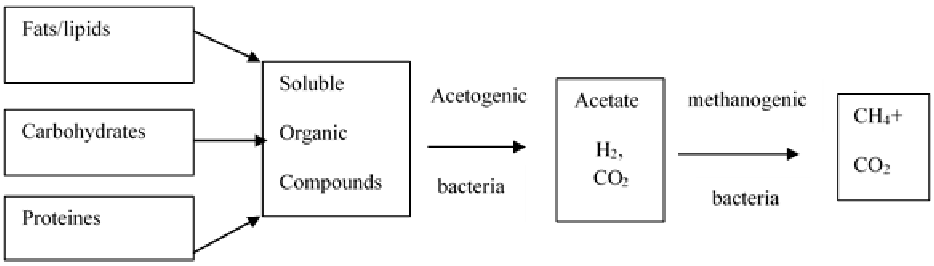

Figure 1. Biochemical process of the anaerobic digestion in 2 phases

For the growth process, we shall consider the function of Monod μ_1 for acidogens bacteria and the function of Haldane μ_2 for methanogens bacteria.

$$\mu_1 = \mu_{1\max}\frac{s_1}{s_1 + K_{s1}}$$

with $\mu_{1\max}$ represents the maximal growth rate and K_{s1} the constant of half–saturation.

$$\mu_2 = \mu_{2\max}\frac{s_1}{s_2 + K_{s2} + \frac{S_2^2}{K_{L2}}}$$

with $\mu_{2\max}$ the maximal growth rate, K_{s2} the constant of saturation and K_{L2} the constant of inhibition.

Equations of the dynamic model

The mathematical model AM2 based on the laws of growths involves the following dynamical variables:

– X_1 concentration of the acidogen bacterial population.
– X_2 concentration of the methanogen bacterial population.
– S_1 concentration of the substratum of carbon materials.
– S_2 concentration of the substrate of AGV

For a batch bioreactor, the mathematical model expresses as a system of coupled differential equations of the first order is:

$$\frac{dX_2}{dt} = \mu_2 X_2, \quad \frac{dS_1}{dt} = -k_1 \mu_1 X_1 \text{ and}$$

$$\frac{dS_2}{dt} = k_2 \mu_1 X_1 - k_3 \mu_2 X_3$$

The methane flow which is the end product directly depends on the growth of the bacterial methanogen population according to the relation:

$$Q_{ch4} = k_4 \mu_2 X_2$$

We distinguish 9 parameters which intervene in this model $(\mu_{1\max}, K_{s1}, \mu_{2\max}, K_{s2}, K_{L2}, k_1, k_2, k_3, k_4)$.

To solve this system of differential equations, it is also necessary to supply the initial conditions which are the estimations of the initial quantities of the substrates concentrations and of the bacteria in the starting up of the bioreactor: $S_1(0), S_2(0), X_1(0)$ and $X_2(0)$.

Analysis and estimation of the model parameters

The performed bibliographical study is based on numerous references concerning the methanogenesis in the anaerobic bioreactors.

We were interested, in particular, in the works which have used the AM2 model for the simulation of bioreactors.

The growth rate parameters

Numerous authors give the values of $\mu_{i\max}(i = 1, 2)$ as cited in the references presented in Table 1 according to the models of Monod and Haldane [KIELY *et al.*, 1997; MULLER *et al.*, 2002; SIMEONOV *et al.*, 2009; NAKHLA *et al.*, 2006; SIMEONO *et al.*, 1996; SIEGRIST *et al.*, 1993; LUBENOVA *et al.*, 2002 ; HUSAIN *et al.*, 1998; HILL *et al.*, 1977; GERBER *et al.*, 2008]. On the other hand, for these authors, they do not supply the values of the parameters K_{Si}.

Table 1.

Comparative table of $\mu_{1\max}$, $\mu_{2\max}$ for various substrate

parameters			
$\mu_{1\max}$ (1/day)	$\mu_{2\max}$ (1/day)	substrate	references
0.6	0.4	Wastewater	[MULLER *et al.*, 2002]
0.4	0.4	Organic waste	[SIMEONOV et al., 2009]
0.25	0.66	For DAF pretreated Waste water	[NAKHLA *et al.*, 2006]
0.55	0.4	Cattle manure	[SIMEONO *et al.*, 1996]
0.3	0.6	Codigesting municipal solid waste and big slurry	[KIELY *et al.*, 1997]
0.55	0.55	Biodegradable solid organic	[SIEGRIST *et al.*, 1993]
0.2	0.25	organic waste.	[LUBENOVA *et al.*, 2002]
0.31	–	Biodegradable volatile solids	[HUSAIN 1998]
0.4	–	Animal waste	[Hill *et al.*, 1977]
0.4	–	Organic Substances	[Gerber *et al.*, 2008]

Table 1 presents the growth rates $\mu_{1\max}$, $\mu_{2\max}$ given by eleven authors working in an environment constituted by waste water under various experimental conditions in batch and continuous bioreactors.

Considering the various conditions, we notice that the growth rates for $\mu_{1\max}$ and $\mu_{2\max}$ remain limited in a range going from 0.2 /day to the 0.66 / day.

On average, both types of bacteria have approximately growth rates $\mu_{i\max}(i = 1, 2)$ comparable and of the order of 0.4 / day. We can also notice that some authors specify $\mu_{1\max}$ and do not specify $\mu_{2\max}$.

For other authors who have used as substrate the glucose and the amino acids, some growth rates go from 5/day to

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Banat's Journal of Biotechnology
2020, XI(22)

25 / day for $\mu_{1\max}$ and move away clearly from average values quoted in Table 1.

Table 2.
The parameters K_{S1}, K_{S2}, K_{L2} of the model AM2

$K_{S1}\left(mg/l\right)$	$K_{S2}\left(mg/l\right)$	$K_{L2}\left(mg/l\right)$	Substrate/ condition	Reference
27.6*	4.13*	17.2*	Waste water	[KIELY *et al.*, 1997]
25.34*	23.47*	48*	food wastewater for DAF–pretreated	[NAKHLA *et al.*, 2006]
14.262*	39.220*	48*	food wastewater for raw wastewater	[NAKHLA *et al.*, 2006]
150*	25*	300*	Poultry farming (25°C)	[Hill *et al.*, 1977]
160*	0.82*	–	Cattle manure (34°C)	[SIMEONO *et al.*, 1996]
500	120	5000	Codig cattle manure (55°C)	[ANGELIDAKI 1999]
300	870	1500	organic waste.	[LUBENOVA *et al.*, 2002]
1805	64	–	Pig manure (20°C)	[MASSE *et al.*, 2000]
22	–	–	Amino acids sugars (35°C)	[BRYERS 2000]
–	500	–	Acetic acid (35°C)	
–	80	–	Acetic acid (35°C)	[TSCHUI 1989]
1.2	1.9	0.41	Caffeic Acid phenolic	[PIANNA *et al.*, 2009]
–	30	–	Acetic acid (35C°)	
50	–	–	Aminoacidic, sugar 35°C	[SIEGRIST *et al.*, 1993]
200	–	–	Long chain fatty acid (35°C)	
2000	–	–	Long chain fatty acid 35°C	[TSCHUI 1989]
23	–	0.8	Glucose (37C°)	[MOSEY 1983]

* Indicate the values used for the average estimation of the parameters.

On the other hand, for methanogens, the $\mu_{2\max}$ rate does not move away from values of Table 1 [KIELY *et al.*, 1997; MULLER *et al.*, 2002; SIMEONOV *et al.*, 2009; NAKHLA *et al.*, 2006; SIMEONO *et al.*, 1996; SIEGRIST *et al.*, 1993; LUBENOVA *et al.*, 2002].

Estimation of K_{S1}, K_{S2} ***and*** K_{L2}

For various substrates, Table 2 presents the $K_{Si}\left(i=1,2\right)$ parameters as given by some authors.

Table 3.
The parameters k_1, k_2 and k_3 of the model AM2 for various substrate and different authors

kinetic parameters	The values	Substrate	Reference
	5	Poultry farming (25 °C)	[HILL *et al.*, 1977]
	37.8	Cattanure sugars	[SIMEONO *et al.*, 1996]
k_1	5.31	Codigesting municipal solid waste and pig slurry (36 °C)	[KIELY *et al.*, 1997]
	4.38	Pig manure (20 °C)	[MASSE *et al.*, 2000]
	14.28	Different animal wastes, pig beef, dairy, poultry sugars (34 °C)	[HUSAIN 1998]
	2.45	Poultry farming Amino acids sugars (25 °C)	[Hill *et al.*, 1977]
	45.51	Cattle manure (34 °C)	[SIMEONO *et al.*, 1996]
k_2	3.543	Codig cattle manure with glycerol trioleate or gelatin	[ANGELIDAKI 1999]
	9	Different animal wastes, pig beef, dairy, poultry sugars (34 °C)	[HUSAIN 1998]
	0.38	Codigesting municipal solid waste and pig slurry (36 °C)	[KIELY *et al.*, 1997]
	16.66	Poultry farming Amino acids sugars (25 °C)	[Hill *et al.*, 1977]
	41.32	Cattle manure (34 °C)	[SIMEONO *et al.*, 1996]
k_3	12.5	Codigesting municipal solid waste and pig slurry (36 °C)	[KIELY *et al.*, 1997]
	23.88	different animal wastes, pig beef, dairy, poultry sugars (34 °C)	[HUSAIN 1998]
	19	Pig manure	[MASSE *et al.*, 2000]

The values of the parameter K_{S2}, are very scattered and vary in an interval of 30 until 500 mg/l and it is true for the same substrate (acetic acid) and the same conditions of temperature.

We also note the absence of some estimation of the parameters K_{S1} or K_{S2} for some authors.

To establish the estimation of the average parameters, we made a selection of the values from Table 2 while eliminating those who in simulation give inacceptable results.

Estimation of k_1, k_2 and k_3 parameters

Table 3 presents the values of k_1, k_2 and k_3 parameters for various substrates. We notice that, for different authors, the parameters k_1, k_2 and k_3 are scattered even when the used substrate remains practically the same.

Table 4.

The k_4 parameter of for various substrate and different authors

kinetic parameters	The values	Substrate	Reference
$k_4\left(l^2/mg\right)$	75*	Waste water	[MULLER *et al.*, 2002]
	74.54*	Cattle manure	[SIMEONO *et al.*, 1996]
	19.5*	Waste waters from different types of animal farming big beef, dairy, poultry	[TSCHUI 1989]
	16.74	Acetic acid	[BRYERS *et al.*, 1985]
	15.37	Acetic acid	[HUSAIN 1998]

* Indicate the values used for the average estimation of k_4

Estimation of k_4 parameter of the methane production

Table 4 presents the estimation of the production parameter of methane k_4 for the AM2 model for various substrate and different authors.

We note that very few authors give an estimation of the k_4 factor.

However, the latter varies in an interval from 19.5 to 75 l^2/mg and it is true for the waste water.

On the other hand, if we use acetic acids as substrate, the value of the parameter k_4 stabilizes around 16 l^2/mg.

Estimation of the initial values of substrate and biomass

Most of the authors do not specify the initial values of the substrate and the biomass concentrations.In the explored bibliography, a single author supplied these values (Table 5).

Table 5.

The initial values of substrate and biomass

The values (mg/l)	Substrate	Reference
$S_1(0)^*$	14–24	[NOYKOVA *et al.*, 2002]
$X_1(0)^*$	0,1	
$S_2(0)^*$	3	
$X_2(0)^*$	0,01	

We note a relationship of substrate / biomass of the order of some percent.

Also, the relationship between the initial concentration of the substrate and of the initial biomass concentration is not highlighted [STOLERU, *et al.*, 2014, CARUSO, *et al.*, 2019. BUTNARIU, *et al.*, 2016].

Estimation of the "average" parameters and simulation

This section will present an estimation of the average parameters which will serve to simulate the functioning of virtual bioreactors by means of the AM2 mathematical model.

A qualitative comparison of the methane production is carried out with the results presented by various authors.

Estimation of the average parameters

The average values of the model parameters estimated with respect to the values given by some authors who used practically the same environment / substrate are presented (Table 6).

Table 6.

The average values for the estimation of the various parameters

The parameters	The average values	The units
$\mu_{1\max}$	0.4	$1/j$
$\mu_{2\max}$	0.4	$1/j$
K_{S1}	72	mg/l
K_{S2}	18	mg/l
K_{L2}	103	mg/l
k_1	13	su
k_2	12	su
k_3	22	su
k_4	56	l^2/mg
S_1	19	mg/l
X_1	0.1	mg/l
S_2	3	mg/l
X_2	0.01	mg/l

Simulation

A simulation was performed by using the "average" parameters of the AM2 model given in Table 6.

An example of result of simulation allowing to visualize graphically the temporal evolution of the substrate and of the methane is presented in Figure 2.

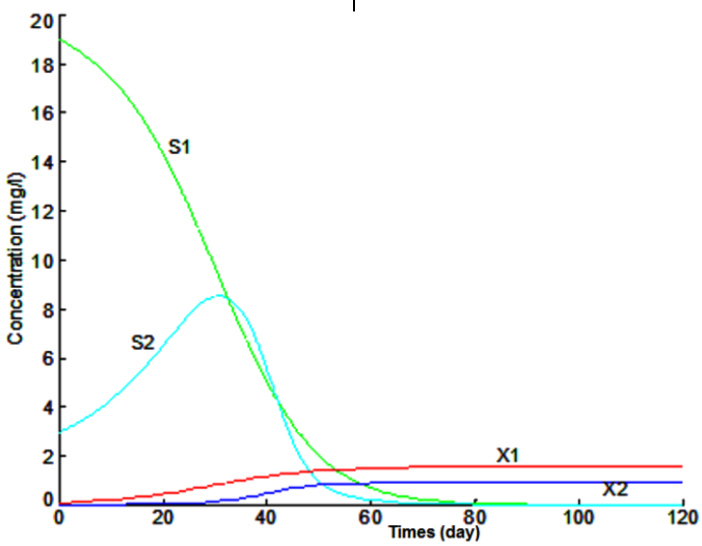

Figure 2. Temporal evolution of substrate and bacteria

We notice for the used values of parameters that there is practically an exponential decrease of the S_1 substrate which will be exhausted in about 80 days.

At the same time, the S_2 (AGV) substrate begins to be generated during the first days and reaches a maximal value in about 35 days then will begin its decrease [BUTU, *et al.*, 2014c, CAUNII, *et al.*, 2015].

This substrate will be practically totally decomposed into biogas in about 70 days [BUTU, *et al.*, 2014b, IANCULOV, *et al.*, 2004].

After consumption of the substrate over a period of about two months, the concentrations of acetogens and methanogens bacteria stabilize in constant values and the mathematical model does not plan their later evolution.

Comparison of the results concerning Methane production

For the methane production, the literature supplies practically comparable data for the k_4 parameter which is estimated in our case by the value $k_4 = 56\, l^2 / mg$ [BUTNARIU, *et al.*, 2015, BUTU, *et al.*, 2014a].

Considering this value, the profile of flow methane $Q(t)\,(liter/day)$ and its accumulation $C(t)$ in liters are represented in Figure 3.

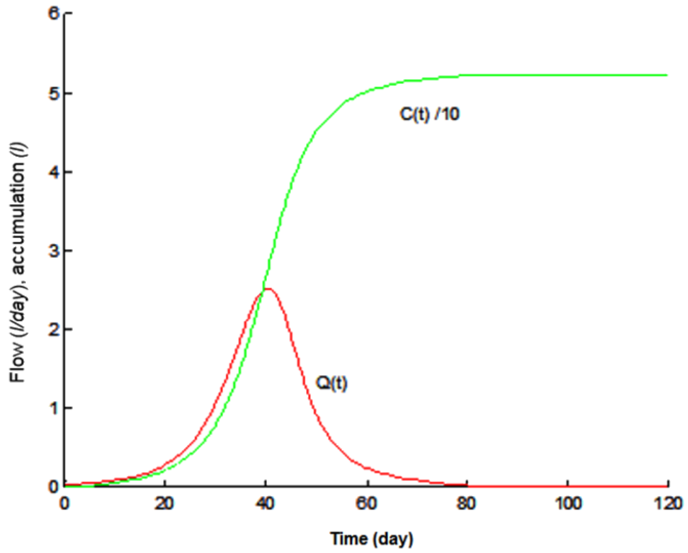

Figure 3. Temporal evolution of methane production

We notice that the scale of *C(t)* was reduced by a factor 10 and that the curve Q shows a fast increase from the beginning of the launch of the bioreactor then reaches a maximum in about 40 days then begins to decrease until nullifying after a duration of 80 days. This type of behavior is the one which is expected for a batch bioreactor.

Table 7.

Maximal duration of the methane production

Maximal duration of production of the methane (days)	The references
15– 20	[BLANCO *et al.*, 2010]
50–70	[ZHANG *et al.*, 2008]
70	[VAVILIN *et al.*, 2002]
9	[ALDIN 2010]
20	[NOPHARATANA et al., 2007]
35	[MOSEY 1983]
14	[CHOI *et al.*, 2003]
70	[JONES *et al.*, 2008a]
15–20	[CHEN *et al.*, 2010]
40	[heo *et al.*, 2004]
20– 30	[DOCHAIN *et al.*, 2008]

For a choice of the model parameters based on the average values, we note a good qualitative correspondence of the profiles obtained by our simulation in comparison with experimental results as well as the simulation results presented by several references among which [MOSEY et al., 1983; VAVILIN et al., 2002 ; SHANMUGAM et al., 2009; BLANCO et al., 2010; ZHANG et al., 2008; CHEN et al., 2010; JONES et al., 2008; DEARMAN et al., 2007; ALDIN 2010; NOPHARATANA et al., 2007; CHOI et al., 2003; DOCHAIN et al., 2008; FANG et al., 2008: SIMEONOV et al., 2000; SORBA 2008; MORAU et al., 2010; ESCUDIE et al., 2005].

Table 7 indicates the necessary durations so that the methane production reaches its maximal value for every cited reference [BUTNARIU, 2014, PETRACHE, et al., 2014].

We shall note that the average value for which the methane reaches a maximal production is about 34 days which remains lower than the duration obtained by our simulation (approximately 40 days).

Conclusions

The simulation of anaerobic batch bioreactors dedicated for the production of methane by means of a developed program according to the mathematical model AM2, shows a strong sensibility of the results (variation of substrates, evolution of bacteria, and production of the methane) with respect to the variations of the model parameters.

To highlight this sensibility, we have undertaken a vast bibliographical analysis which have confirmed actually a serious dispersion in the estimation of the model parameters as given by many authors.

On the other hand, we have also noticed that only few researchers have supplied the values of these parameters, in their papers.

An estimation of the "average" parameters of the model based on the bibliography was derived and has allowed to simulate the functioning of the bioreactor with these data. A comparative analysis of this model for different parameters was carried out. Following our analysis of this problem, we consider that the AM2 model renders qualitatively the functioning of the batch bioreactors. However, the model needs to be more deeply studied theoretically and experimentally to highlight the sensibility of the model parameters with respect to the biological, biochemical and physical factors influencing the bioreactors.

More elaborate studies should be led to determine at least the domain of variation of the model parameters in regard to the used substrate and to the experimental conditions.

Conflict of Interest: The authors declare that they have no conflict of interest.

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