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Study of a theoretical approach to bioprocess modeling for the performance of an anaerobic digester

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Abstract

Anaerobic digestion represents one of the major challenges of sustainable development and circular economy in the concept "from waste to energy". Given the great diversity of organic waste, its development requires the optimization of co-digestion. Hence the need to develop simple tools to characterize substrates and to predict the performance of digesters in order to optimize their operation. In this work, an approach based on a simple mathematical model to be able to calculate the biogas yield was studied. The models studied (AM2 and ADM1), serve as a basis for the development of monitoring and regulation strategies, offering more or less detailed levels of description of the digestion process. We have identified a difference in complexity between these two models explained by the different objectives for which they were developed. Thus, our study aims to propose a theoretical approach to the modeling of bioprocesses by choosing between the two aforementioned models. The objective being to provide a certain ease to the biogas producer and designer of digesters in the rural world, the simple model chosen is justified by intermediate stages of lesser importance than the final stage of methanogenesis. Thus, the information collected and estimated can subsequently be used for control strategies to optimize the operation of the digester, or they can be used by monitoring and diagnostic systems. This model will give a synthetic vision of anaerobic digestion, which limits its use to the modeling of the treatment of simple effluents. On the other hand, its formulation will allow a thorough mathematical analysis, and its simple structure would be well suited to the development of control strategies or monitoring procedures.

Keywords: Anaerobic Digestion; Mathematical Model; Modeling of Bioprocesses; Biogas

1. Introduction

The performance of an anaerobic digester is closely related to the structure of the microbial community present depending on the type or mechanism of the bioprocess of the system. "Bioprocess" is a term used to generally designate systems for treating municipal and industrial waste and wastewater by biological means. The principle consists in using microorganisms in contact with organic matter in order to degrade it, and this, in basins where the environmental conditions are maintained appropriate. Two main types of bioprocesses are distinguished and can be considered as potential candidates for treating wastewater: aerobic systems operating in the presence of oxygen and anaerobic systems, where microorganisms can only develop in the absence of oxygen. The technique used in anaerobic systems is called anaerobic digestion or methanization. It is a complex process involving several biological reactions. It is generally described by four main steps: hydrolysis, acidogenesis, acetogenesis and methanogenesis, involving four specific microbial consortia interacting with each other. Each of the steps is carried out by populations of complex microorganisms which, under specific and regular environmental conditions and substrate supply, form stable communities [1-2].

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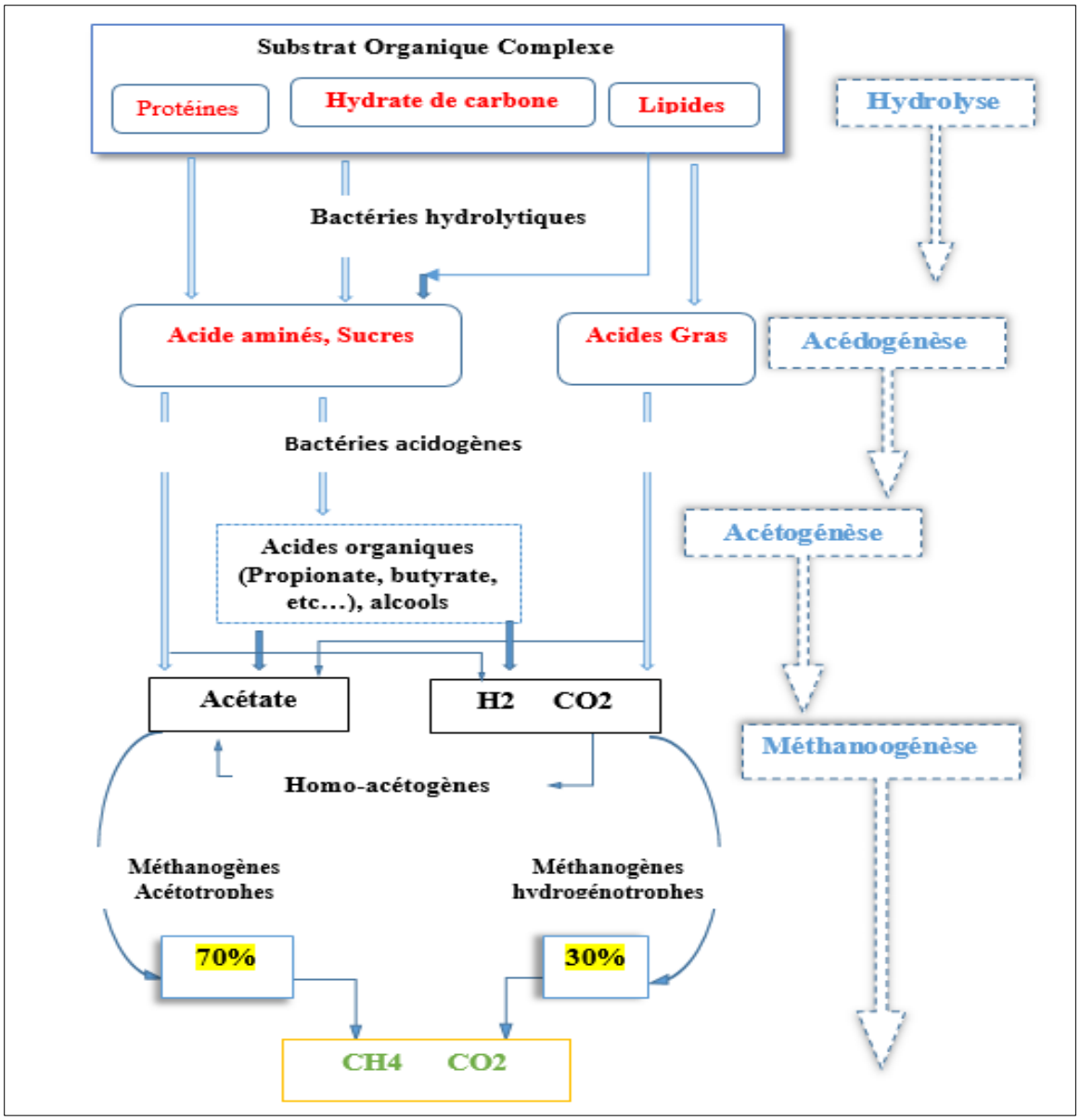

Figure 1 Simplified steps of the anaerobic digestion process

Normally in anaerobic digestion, all the steps of the process are carried out in the same digester. Many authors have demonstrated the advantages of two-stage anaerobic digestion compared to conventional single-stage anaerobic digestion [3-6].

However, the main advantage of anaerobic digestion is the possibility of producing energy in the form of biogas contained in methane. But the start-up of this process is slow and its operation can be destabilized by disturbances. How then can we ensure the stability of methanizers over time, improve their treatment efficiency and optimize methane production, despite environmental disturbances and variations in key process parameters?

Manual control based on knowledge from process expertise can be a first answer to our question. Unfortunately, this solution has two drawbacks:

- It is difficult to ensure optimal operation in this way.
- Detecting destabilization following a possible overload is not always easy. It requires the operator to constantly monitor the various quantities and variables and in many cases, the first signs of destabilization are not detected.

These disadvantages, which can be costly in economic terms, lead designers and users to propose the implementation of automatic control of the biological process. For this, like any other industrial process, bioprocesses need to be modeled, supervised, diagnosed and controlled: this is how bioprocess automation appeared in the 1980s, made possible by the development of sensors and computer systems.

By dividing anaerobic digestion into two stages, we promote conditions and an environment conducive to specialized microorganisms for each of the stages of anaerobic digestion [7].

During the operation of an anaerobic digestion process, the major problem comes from the fact that Volatile Fatty Acids (VFA) produced during the acidogenesis reaction can accumulate in the bioreactor and thus destabilize the process. This is the reason why modeling, control and supervision tools are necessary to optimize the operation of anaerobic digesters.

According to the objective for which they were developed, anaerobic digestion models can be classified into two groups: i) large-scale models, developed by practitioners to reproduce the phenomenological behavior of the system and ii) simplified models developed for control, describing macroscopically anaerobic digestion in a small number of cascade steps and having a limited dimension. A state of the art on anaerobic digestion models existing before 1999 is given in [8].

Appearing at the end of the 1990s, the modeling of anaerobic digestion processes constitutes an important research axis since it allows to integrate in a single tool all the knowledge acquired on the internal and/or external functioning by taking into account the entire environmental system or one studies, that is to say the bio-physico-chemical digestion environments. The modeling aspect remains however a powerful tool of dynamic simulation, of the digestion environments which can be used in a wide spectrum of applications linked on the one hand to the entire dimensioning of the anaerobic digester. This involves:

- Understanding of complex phenomena;
- Determination of certain kinetic parameters difficult to access by experimentation;
- Prediction of the kinetics of degradation, dynamic evolution of the environments;
- Optimization of the yield in quantity and/or quality according to the needs;
- Rapid comparison of different parameters (organic load, residence time, substrate, etc.)

In most of the bibliographic literature that we have used, the objective of the modeling remains in the concept of sizing and/or optimizing a yield, therefore most of it methane CH_4. In either case or in the combination of the two cases there is always the integration of one of the elements mentioned above.

2. Materials and Method

2.1. Presentation of the models studied

To carry out our work, we will study the state of the bibliographic art of the two models

The characterization of the physicochemical composition of the substrates is an important step in the modeling, monitoring and control of bioreactors.[9]

We will study the case of the model of a biodigester proposed by: [10]

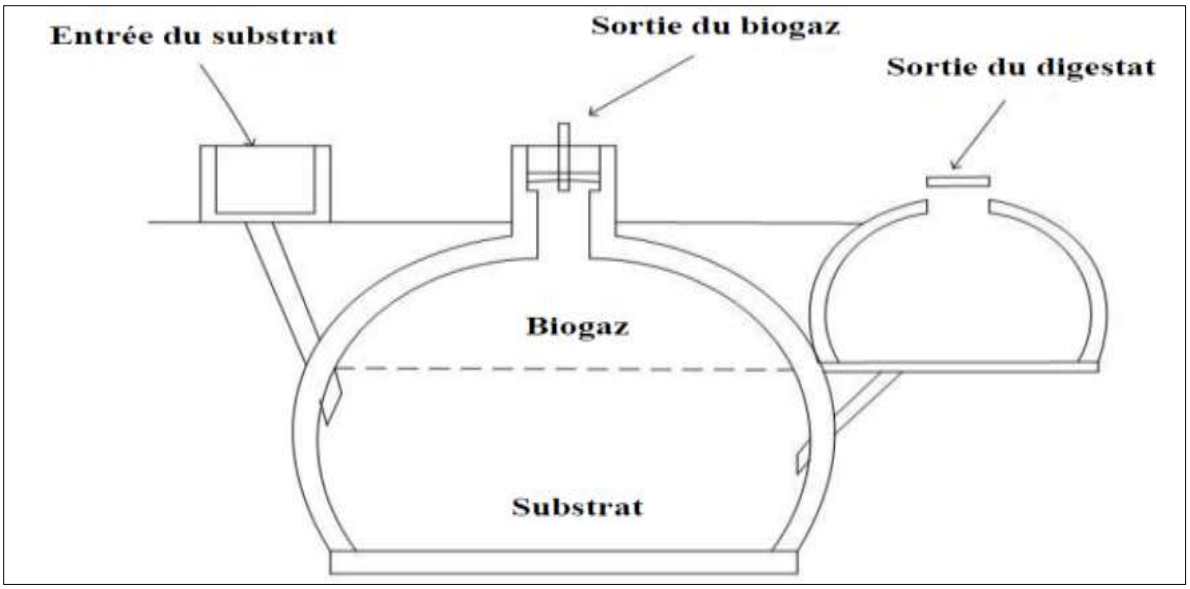

Figure 2 Diagram of the anaerobic digester studied by [10]

The table below presents in a synthetic way the differences in complexity of the AM2 and ADM1 models

Our objective being to model the production of biogas, and more particularly the production of methane, the intermediate stages are of lesser importance than the final stage of methanogenesis. Furthermore, Bernard et al. (2006a) [12] have shown that in many cases, models as simple as the Andrews model (1968) [13] were sufficient to correctly predict a certain number of variables.

2.2. Study of the enzyme kinetic model

The foundations of microbial kinetics derive from enzyme kinetics in Chemistry. Despite non-ideal experimental conditions (unbuffered medium, use of unpurified enzymes), the first research in this field highlighted the catalytic role of enzymes through Enzyme-Substrate complexes [14]. A first essential step was taken when a mathematical model was proposed to describe the rate of an enzymatic reaction v as a function of the substrate s:

$$v = V_m \frac{S}{K_s + S}$$

where Vm is the maximum reaction rate and Ks is the concentration at which the rate is half the maximum. This relationship, initially proposed by Victor Henri in 1902, known as the Michaelis-Menten relationship, has been confirmed many times since its introduction [15].

A few years later, around 1925, John B. S. Haldane and George Edward Briggs proposed a different interpretation of Henri's work and introduced an equation representing the inhibition of an enzymatic reaction by an excess of substrate:

$$v = V_m \frac{S}{K_s + S + \frac{S^2}{K_i}}$$

where Ki is the inhibition constant

In the literature, several authors do not take into account the aspect of inhibition due to the presence of inhibitors preventing part of the reactions from operating correctly.

The first convincing model linking the bacterial growth rate μ to a limiting substrate s was introduced by Monod (1942) [16] who proved that the slowing down and stopping of bacterial growth is linked to the depletion of substrate in the culture medium.

From the mass balances he had obtained, he suggested that bacterial growth be represented by a two-parameter function μm and Ks according to the equation:

$$\mu = \mu_m \frac{s}{K_s + S}$$

where the parameter ks represents the affinity of microorganisms for the substrate, and μm the maximum growth rate. Although this model is close to the Michaelis-Menten equation for enzyme kinetics, Monod only made the connection later, around 1950, when discussing the role that enzymes play in substrate degradation. Monod also formulated the principle that the growth rate of a bacterial population could always be represented as the product of the living biomass x, and another factor μ which would be the growth rate (Monod, 1942) [16]:

$$\frac{dx}{dt} = \mu x$$

He subsequently developed the first chemostat model (A chemostat is a laboratory device (of the bioreactor type) in which organisms (bacteria, phytoplankton) grow in a controlled manner). He presented the conservation equations of two variables, the biomass concentration (density) x and the limiting substrate s, in a continuous bioreactor by considering the "sources" and "sinks" for these quantities, and he proposed the following system to describe their evolution:

$$\begin{cases} \frac{ds}{dt} = -Dx + \mu(s) \\ \frac{dx}{dt} = D(s_{in} - s) + \frac{\mu(s)}{Y} x \\ \mu(s) = \mu_m \frac{s}{k_s + s} \end{cases}$$

where Y denotes the efficiency of substrate conversion to biomass, and S_{in} is the concentration of organic substrate in the chemostat feed. The dilution rate D is defined as the ratio of the feed flow rate Qin to the reactor volume Vl:

$$D = \frac{Q_{in}}{V_l}$$

This system not only allows the determination by integration of the equations of evolution of the variables, but the study of the equilibria of the system shows that the growth rate can be imposed (to a certain extent) through the dilution rate; in fact the first equation is reduced to equilibrium to the following equality:

$$D = \mu(s)$$

The first macroscopic descriptions of the phenomenon concerning the modeling of fermentation processes, date back to the beginning of the 20th century with the general equation of the degradation of organic matter by fermentation [2 ; 17] which allows, knowing the characteristics of the food, to predict the products formed.

$$C_nH_aO_b + \left(n - \frac{a}{4} - \frac{b}{2}\right)H_2O \rightarrow \left(\frac{n}{2} - \frac{a}{8} + \frac{b}{4}\right)CO_2 + \left(\frac{n}{2} + \frac{a}{8} - \frac{b}{4}\right)CH_4$$

Since fermentation is a complex process, the choice of reactions to represent constitutes the first step in the construction of the mathematical model, and then the equations of evolution of the different variables must be obtained. Despite the absence of universal laws for bacterial kinetics, principles such as the conservation of matter, or electroneutrality apply to bioprocesses. The use of mass balances constitutes a powerful tool for deducing the equations of the model[18-20]. The evolution of the mass M of a constituent is defined by the following equation:

$$\frac{dM}{dt} = \underbrace{M_{Entrées} - M_{Sorties}}_{Flux\,entrée/Sortie} + \underbrace{M_{Gaz \rightarrow Liquide} - M_{Liquide \rightarrow Gaz}}_{Echanges\,gazeux} + \underbrace{M_{Produite} - M_{Consommée}}_{Bioréaction}$$

A large number of models are based on this method, and the differences are mainly in the choices of representation of bacterial kinetics.

The first models focused mainly on methanogenesis under the hypothesis that it would be the limiting step in the overall anaerobic digestion process. Andrews (1968) proposed to use a Haldane function as the equation system that follows, to represent the inhibition of the growth of methanogens at high substrate concentrations. He studied the system in the case of a closed culture (D = 0) and a continuous culture.

$$\begin{cases} \dfrac{ds}{dt} = -Dx + \mu(s)x \\ \dfrac{dx}{dt} = D(s_0 - s) + \dfrac{\mu(s)}{Y}x \\ \mu(s) = \mu_m \dfrac{s}{k_s + s + \dfrac{s^2}{k_i}} \end{cases}$$

He linked the unstable nature of anaerobic digestion to the existence of two locally stable equilibrium points for this system. He also highlighted the idea of "leaching" and maximum dilution rate, i.e. the dilution rate beyond which the residence time in the bioreactor is lower than the growth rate, and does not allow the accumulation of biomass. In 1973 a complete model considering only one bacterial species, methanogens, was presented by Graef and Andrews. By considering an empirical molecular formula of bacterial biomass (C5H7NO2), they obtained a stoichiometric equation representing the conversion of acetate into biogas and biomass:

$$CH_3COOH + 0,032NH_3 \rightarrow 0,032C_5H_7NO_2 + 0,92CO_2 + 0,92CH_4 + 0,096H_2O$$ interested in non-competitive inhibition of growth on a simple substrate, Ierusalimsky introduced the following equation where I is the concentration of the inhibitor and Ki the inhibition constant:

$$\mu = \mu_m \frac{s}{K_s + s} \frac{K_i}{K_i + I}$$

The consideration of the solubilization of organic compounds in a general model of anaerobic digestion was determined by Sinechal et al. in 1979 [21]. Subsequently, the representation of the process was improved by considering additional steps. Other authors have been interested in the inhibition by substrates other than VFAs, such as nitrogen (Hill and Barth, 1977) [22], hydrogen by (Mosey, 1983) [23] or sulfated compounds (Kalyuzhnyi et al., 2000a) [24]. The authors Hill and Barth include an additional term in the Haldane equation of the growth rate of methanogens to represent the double inhibition by VFAs and dissolved ammonia (NH3) in the digestion of livestock effluents:

$$\mu = \mu_m \frac{agv}{agv + K_s + \dfrac{agv^2}{K_i + \dfrac{NH_3 \cdot agv}{K_n}}}$$

3. Result and Discussions

3.1. Theoretical result of the AM2 Model of two-stage anaerobic digestion

The two-stage AM2 model is a simple model to identify, capable of reproducing the dynamic behavior and taking into account the phenomenon of destabilization of anaerobic digesters by accumulation of Volatile Fatty Acids (VFA). This mass balance model is derived from the model for the infinitely mixed reactor presented in Bastin and Dochain (1990), but it introduces an additional parameter that allows to account for the attachment of biomasses on the digester support. Of all the current models, it appears as one of the most suitable for the control of these systems. Subsequently, it was developed within the framework of the European AMOCO project, on the modeling and control of anaerobic digestion processes.

The development of the AM2 model is based on the hypothesis that the bacterial populations involved in anaerobic digestion can be divided into two main groups of homogeneous characteristics and that anaerobic digestion can be described by a two-stage process and only two substrates and two bacterial groups are considered. In the first step called acidogenesis, the consortium of acidogenic bacteria (X1) transforms organic matter (S1) into VFA (S2) and carbon dioxide CO2. In the second step called methanogenesis, the population of methanogens (X2) converts S2 into methane CH4 and CO2.

1. Acidogenesis, with a reaction rate r1 = μ1(S1) X1, such that μ1(S1) is the specific growth rate of X1 on S1:

2. Methanogenesis, with a reaction rate r2 = μ2(S2)X2, such that μ2(S2) is the specific growth rate of X2 on S2:

$$\text{Acidogénèse}: \quad k_1 s_1 \xrightarrow{r_1} X_1 + k_2 s_2 + k_4 CO_2$$

$$\text{Méthanogénèse}: \quad k_3 s_2 \xrightarrow{r_2} X_2 + k_5 CO_2 + k_6 CH_4$$

Here the production and consumption of hydrogen during the overall process are not represented. The growth kinetics of acidogenic bacteria is represented by the Monod equation $\mu_1(S_1) = \overline{\mu_1} \dfrac{S_1}{S_1 + K_{S1}}$

whereas the inhibition of methanogen growth by high concentrations of VFAs obeys Haldane kinetics

$$\mu_2(S_2) = \overline{\mu_2} \frac{S_2}{S_2 + K_{S2} + \frac{S_2^{\,2}}{K_{I2}}}$$

3.2. Mathematical equation of the model

The resulting differential system is written for a fixed bed reactor:

The general two-stage AM2 model as proposed in the literature, considers

6 named state variables:

- S1: The concentration of organic matter to be degraded (COD),
- X1: The concentration of acidogenic biomass,
- S2: The concentration of volatile fatty acids (VFA),
- X2: The concentration of methanogenic biomass,
- Z: The concentration of alkalinity,
- C: The concentration of inorganic carbon.

We consider the state vector ξ = (X_1;X_2; S_1; S_2;) . The variables Z and C can be added later if necessary, in order to synthesize observers for example.

From the reaction schemes of acidogenesis and methanogenesis and using the mass balance law.

: $\dot{\xi} = K\phi(\xi) + D(\xi_{in} - \xi) - Q$ the reduced AM2 model of dimension 4 is then written in the form:

$$\dot{\xi} = f(\xi)$$

$$\dot{X}_1 = (\mu_1(S_1) - \alpha D)X_1$$

$$\dot{S}_1 = D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1$$

$$\dot{X}_2 = (\mu_2(S_2) - \alpha D)X_2$$

$$\dot{S}_2 = D(S_{2in} - S_2) + K_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2$$

Avec les paramètres Z et C

$$\dot{Z} = D(Z_{in} - Z)$$

$$\dot{C} = D(C_{in} - C) - q_c(\xi) + k_4\mu_1(S_1)X_1 + k_5\mu_2(S_2)X_2$$

With: K: the matrix containing the efficiency coefficients (stoichiometric),

ξ_{in} : the vector of the elements entering the bioreactor,,

Q : the gas exchange terms between the gas phase and the liquid phase,,

$\phi(\xi)$: the vector of the reaction rates,

D : dilution rate ([1/j]),

$\alpha \in [0, 1]$: parameter representing the fraction of the biomass that is not retained in the bioreactor

S_{1in} : the concentration of S1 in the feed ([g/l]),

S_{2in} : the concentration of S2 in the feed ([mmol/l]),

k1 : the degradation yield of S1 by X1 ([g/g]),

k2 : the production yield of S2 by X1 from S1 ([mmol/g]),

k3 : the degradation yield of S2 by X2 ([mmol/g]).

μ1(.) et μ2(.) are the kinetics of the system.

3.3. Limitation of the AM2 model

The choice to omit in the AM2 model certain metabolic pathways such as the degradation of amino acids, or acetogenesis and hydrogenotrophic methanogenesis allows to obtain a very synthetic structure. However, this simplicity has a certain price, since this model is limited to simple diets (only 2 substrates).

Table 1 Differences in complexity of the ADM1 and AM2 models according to 10 and 11

	ADM1	**AM2**
Process	Solubilization Hydrolysis Acidogenesis Acetogenesis Methanogenesis	Acidogenesis Methanogenesis
Biomass	7	2
Reactions	19	2
Parameters	86	13
Outputs	32	8

The very large difference between these two models raises the question of the legitimacy and usefulness of a simple model compared to more comprehensive models

In recent years, the level of understanding of anaerobic digestion processes and their representation via mathematical models has increased considerably [25-31]. However, the practical and industrial use of the models has been relatively low. One reason may be the wide variety of models and their often very specific nature. Among the models proposed in the literature, the ADM1 model (Anaerobic Digestion Model no. 1) remains an essential reference [31].

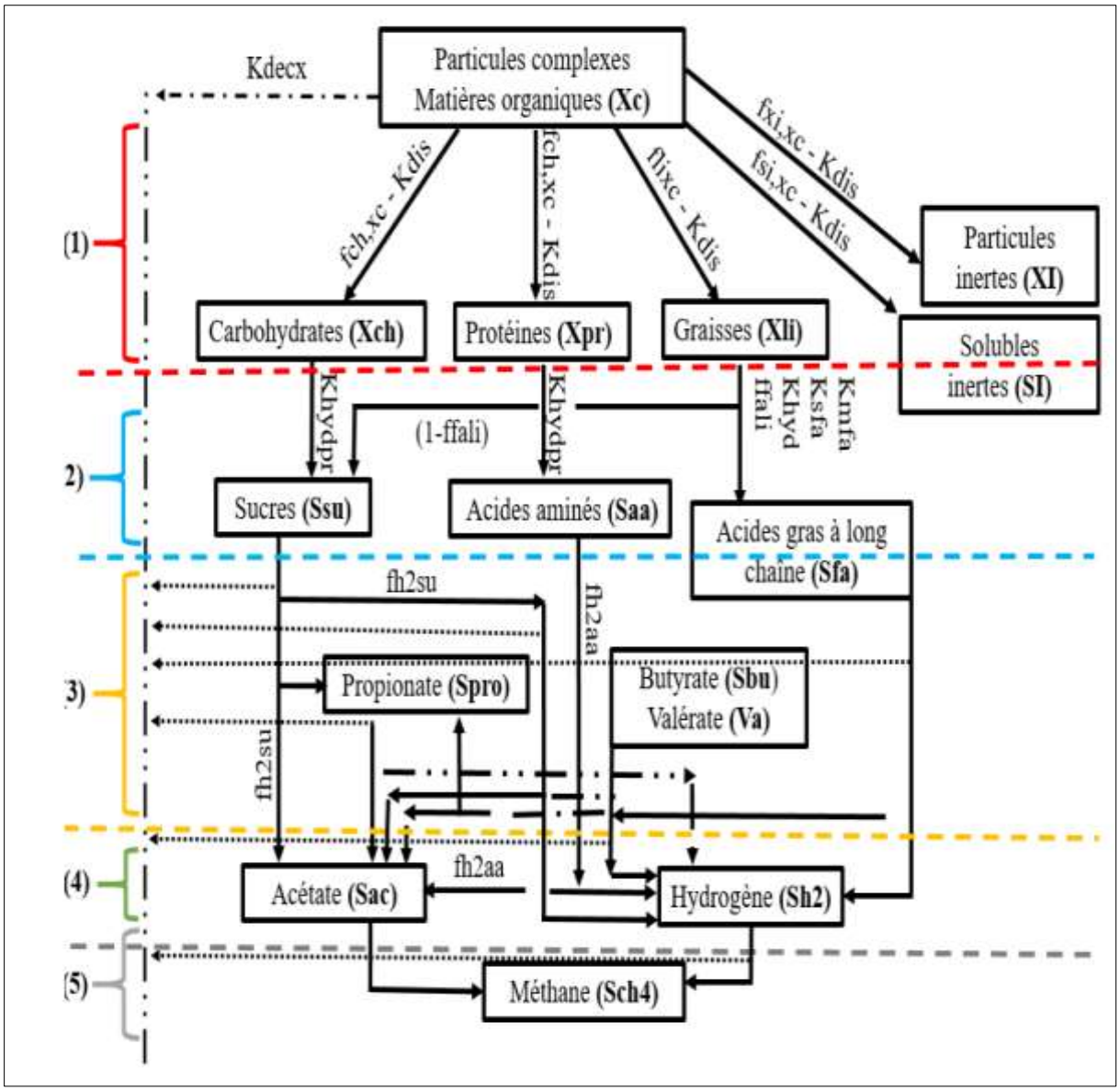

Figure 3 Schematic representation of anaerobic digestion. (1) Disintegration, (2) Hydrolysis, (3) Acidogenesis, (4) Acetogenesis and (5) Methanogenesis. According to [10]

This model from the International Water Association (IWA) aims to propose a generic model, adaptable for different case studies and representative of the anaerobic digestion process. This model is made generic through the use of a nomenclature, units and a structure of coherent and unified equations. It was proposed in 2002 with the aim of providing a common platform for modeling and simulating the different differential and algebraic equations describing the different stages of the anaerobic digestion process in a biological reactor

3.4. Combined result of an approach on the model considered in our work

We define several terms by highlighting a certain number of mathematical tools which, applied to the problem analyzed, will allow us to identify, and quantify, as far as possible, the existing relationships between the characteristic parameters of the biogas generated and the thermal parameters and also understand the characteristics of the ratio used according to the temperature and the influence of the chemical kinetics of the anaerobic digestion process. It will be a question of trying to determine models of the relationships in order to allow a more in-depth exploitation of the data collected on the process.

To identify our model, our objective would not be to describe the mechanisms of the phenomena appearing "inside" the process (for example: the physicochemical relationships), but to represent the behavior of these mechanisms in a relatively less complex way as possible.

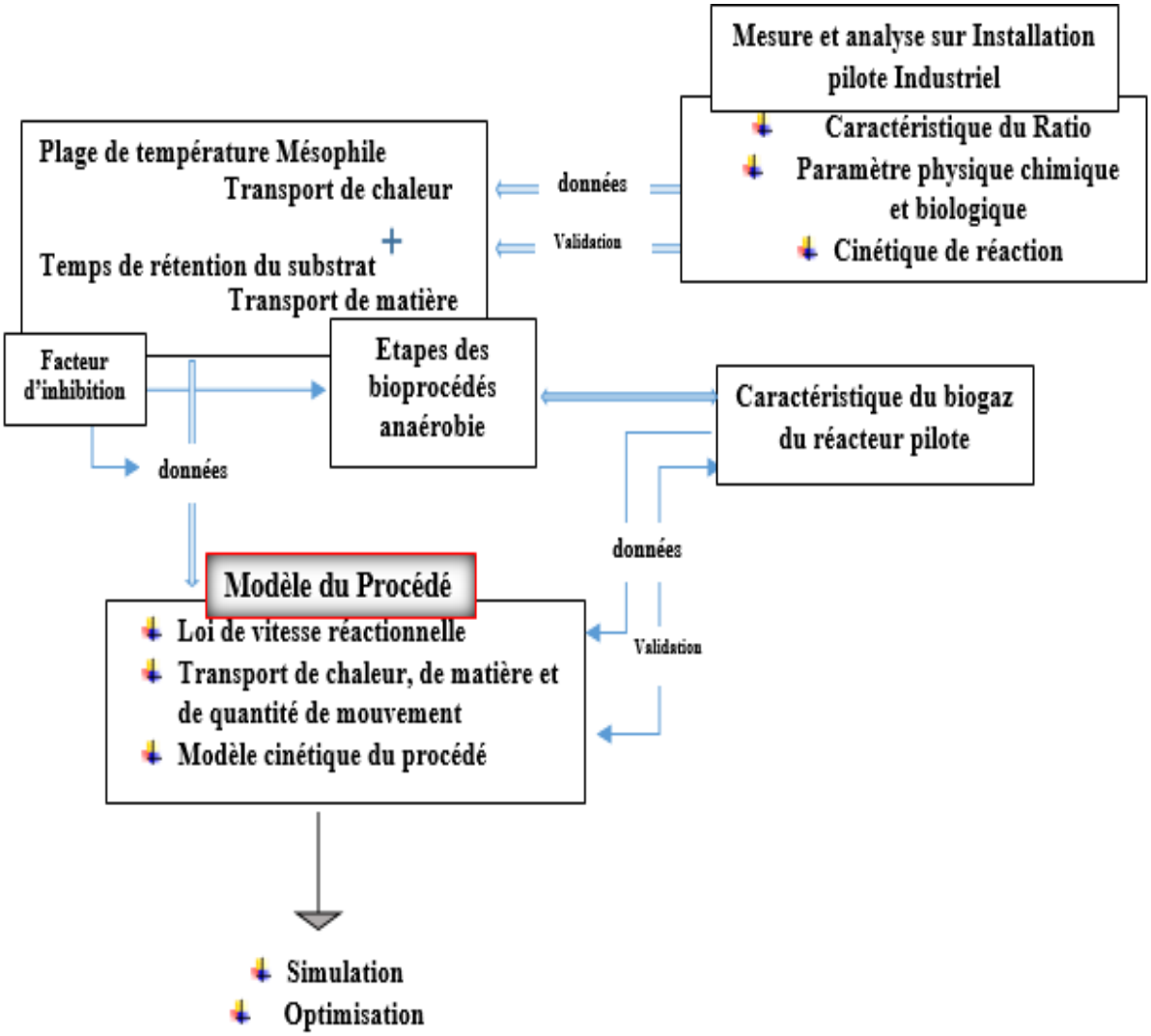

Figure 4 Approach followed for modeling

3.5. Result of the Identification Protocol for a simulation or optimization

We will follow a protocol for identifying models commonly accepted in the bibliographic literature by adapting it to our study context;

- Planning the experiment to collect numerical data and follow the sampling process
- Preparation of the "raw" data in order to clearly highlight the dynamics of the process by calculating the numerical data and comparing with the results in the field
- The dynamics of anaerobic digestion processes play a central role in the development and operations of anaerobic treatment systems.
- For a simulation, we believe that it is necessary to take into account all positive and negative data and analyze them in order to select the best sampling to establish a good optimization.
- To be able to make a good optimization, it is often necessary to list "positive raw data" to minimize imperfections and remove unwanted ones.
- In order to adjust a larger set of sampling measures it is important to have a sufficiently significant number of samples (a few dozen at least) depending on the availability of data and the need.

4. Conclusion

In the same way that one can seek to control a chemical or physical process, research on the modeling of bacterial growth responds to the desire of scientists to understand and describe microbial processes in order to control them.

Monitoring and controlling an anaerobic digestion process under optimal operating conditions is a challenging task due to the complexity of the system and the lack of online sensors for biological and biochemical variables. Mathematical modeling of the anaerobic digestion process is the first step in its automation. A model can be developed for a wide variety of purposes. It can be used to reproduce or explain an observed behavior, to predict a behavior, or to control a system. However, it is only useful if it can answer the questions that are asked about the process studied. It is also characterized by a domain of validity for which the agreement between the model output values and the measurements is satisfactory with regard to the objectives that have been set. The model will be used in a second step to develop simulation models in order to test and evaluate the estimation and control strategies [32-33]. Several models have been proposed in the literature to model the anaerobic digestion process [29-31]. Among the models presented in the literature, the anaerobic digestion model (ADM1) proposed in [15] is probably the most widely used. The ADM1 model, which has become a benchmark, has been tested in several applications such as municipal sewage sludge, solid waste, agricultural waste, livestock waste and crop residues. ADM1 is a structured model that integrates physical, chemical and biological processes. A total of 19 biochemical processes are included, e.g. disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis [31]. For the selection of an appropriate model, this procedure can allow the simultaneous determination of some input state variables of the model and the corresponding hydrolysis kinetics [34]. For this, the model will be identified from the measurement of biogas production (CH4 and CO2), the concentration of chemical oxygen demand (COD) and the concentration of volatile fatty acids (acetate, propionate and valerate) [12].

Compliance with ethical standards

Acknowledgments

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Disclosure of conflict of interest

The authors declare no conflicts of interest.

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