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Theoretical and Numerical Modeling of the Production and Valorization of Biogas Produced by Methanization of Maize Waste in Morocco

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Dedication

This work is dedicated to the memory of my supervisor Professeur Ahmed Mzerd Who has died on 10 december 2021.

We've lose one of the biggest icons here in the faculty of sciences in Rabat which was not easy for all the people who knows him.

For that sad moments I want from the reader of this thesis to pray for him and surely professeur Mzerd will stay in the memory…

Résume

La gestion des déchets devient un défi sérieux qui pousse non seulement le domaine scientifique, mais aussi les gouvernements ainsi que les individus à le relever avec plus de sérieux.

Pour cette raison, de nombreux pays, dont le Royaume du Maroc, se sont engagés dans les nouvelles politiques qui peuvent faire des déchets une source de valeur qui rendra non seulement la planète dans un meilleur état, mais aussi la vie humaine qui est l'essence de cette existence.

Le travail derrière cette thèse était comme une nouvelle fenêtre sur l'utilisation des résidus agricoles en particulier les résidus de maïs, sachant ainsi que la production mondiale de maïs a fortement augmenté, passant de 150 millions de tonnes en 1950 à près de 840 millions de tonnes en moyenne depuis le début de l'année 2010. Les principaux producteurs sont les États-Unis, la Chine, avec une presque égalité du Brésil et l'Union européenne. La France réalise à elle seule environ 25% de la production de l'Union européenne.

Le Maroc, lui aussi, joue un rôle modeste dans la production de plants de maïs notamment dans la région du Grand Casablanca-Settat, suivie de la région de Marrakech-Safi puis de la région de Rabat-Salé-Kénitra. Selon les données publiées par le ministre de l'Agriculture, la production de maïs au Maroc en 2016/2017 dans la région de Casablanca 54898 tonnes a été récoltée sur 56705 hectares.

Ainsi en parlant de gestion des déchets on voit que les résidus de maïs ont une grande part dans ce type de cultures agricoles ce qui nous pousse à réfléchir à l'utilisation de ces grandes ressources de biomasse lignocellulosique qui peuvent devenir une grande source de production de biogaz comme énergie verte ainsi que la planète terre doit maintenir l'équilibre pour les prochaines générations.

La méthode de modélisation adoptée pour cette étude a été réalisée par le modèle le plus complet et intégré au monde des eaux usées qui s'appelle l'ADM 1 qui a été créé par le “Task Group” en 2002. Ce dernier est couplé au modèle hydro-thermique pour les déchets de maïs qui se compose de paramètres de température, d'humidité et d'autres paramètres physiques qui ont un impact important dans cette étude.

Mots clés: Dégradation, digestion anaérobie, modélisation mathématique, déchets de maïs, résidus de cultures, ADM1.

Abstract

Waste management becomes a serious challenge that pushes not only the scientific field but also governments as well as individuals to take it with more seriousness and earnestness.

For that reason, many countries including The Kingdom of Morocco have engaged in new policies that can make waste a source of value that will make not only the planet in a better state but as well as human life which is the essence of this existence.

The work behind this thesis was as a new window to the use of agricultural residues especially the corn residues, so knowing that the world corn production has risen sharply, from 150 million tons in 1950 to almost 840 million tons on average since the start of the 2010s. The main producers are the United States, China, and then practice on an equal footing, Brazil, and the European Union. France alone achieves about 25% of the production of the European Union.

Morocco, as well, has a humble part in the production of maize plants especially in the Grand Casablanca-Settat region, followed by the region of Marrakech-Safi then the region of Rabat-Sale-Kenitra. According to data released by the minister of agriculture, the production of maize in Morocco in 2016/2017 in the region of Casablanca 54898 tons was harvested from 56705 hectares.

So while talking about waste management we see that corn residues have a big part in this type of agricultural crops which pushes us to think about the use of these big resources of lignocellulosic biomass that can become a great source of biogas production as green energy that the planet earth need to maintain the balance for the next generations.

The modeling way adopted for this study was by implementing the most complete and integrated model in the world of wastewater which is called the ADM1 that was created by the Task Group in 2002. This latter is coupled with the hydro-thermal model for the waste of maize which consists of temperature parameters, humidity, and other physical parameters that have an important impact in this study.

Keywords: Degradation, anaerobic digestion, mathematical modeling, maize waste, crops residues, ADM1.

List of Publications and Author's Contributions

Publications in peer-reviewed journals

M A BELLAHKIM, K GUERAOUI, M MAHBOUB, R BELGADA, M TAIBI, G DEBENEST , Application of the IWA Anaerobic Digestion Model (ADM1) for the valorization of maize residues in Morocco, 2019 International Journal on Engineering Applications (IREA), Vol. 7(6):220.

R BELGADA, K GUERAOUI, A. MZERD, M A BELLAHKIM, H. BENBIH. A Biological Degradation Model of Sunflower Waste with Comparison of the Growth Profiles of Microorganisms Between the Meal and the Complete Sunflower Seed, (2020) International Journal on Engineering Applications (IREA), 8 (3), pp. 107-117.

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Communications in international congresses

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Abbreviation and Acronyms

AD	Anaerobic Digestion
LB	Lignocellulosic Biomass
ADM1	Anaerobic Digestion Model no. 1
IWA	International Water Association
MW	Maize Waste
COD	Chemical Oxygen Demand
aa	Amino acids
LCFA	Long-Chain Fatty Acids
H_2	Hydrogen
ac	Acetate
fa	Fatty Acid
c4	Valerate and Butyrate
pro	Propionate
CH_4	Methane Gas
CO_2	Dioxide Carbon
I	inhibition function
$K_{m,process}$	Monod maximum specific uptake rate $kgCOD.m^{-3}$
$K_{S,process}$	Half saturation value $kgCOD.m^{-3}$
S	Substrate concentration $kgCOD.m^{-3}$
S_{ac}	Total acetate concentration $kgCOD.m^{-3}$
S_{bu}	Total butyrate concentration $kgCOD.m^{-3}$
S_{CH4}	Methane gas concentration $kgCOD.m^{-3}$
S_{H2}	Hydrogen gas concentration $kgCOD.m^{-3}$
S_{pro}	Total propionate concentration $kgCOD.m^{-3}$
S_{su}	Monosaccharides concentration $kgCOD.m^{-3}$
S_{va}	Total valerate concentration $kgCOD.m^{-3}$
t	time d
X_{Ch}	Carbohydrates degraders concentration $kgCOD.m^{-3}$
X_{Li}	Lipids degraders concentration $kgCOD.m^{-3}$
$Y_{substrate}$	Yield of biomass on substrate $kgCOD$
Y_{Su}	Yield of biomass on sugars $kgCOD$
Y_{c4}	Yield of biomass on butyrate $kgCOD$
Y_{pro}	Yield of biomass on propionate $kgCOD$
Y_{ac}	Yield of biomass on acetate $kgCOD$
Y_{H2}	Yield of biomass on hydrogen $kgCOD$
$f_{bu,su}$	Yield of butyrate on sugar $kgCOD.kgCOD^{-1}$
$f_{pro,su}$	Yield of propionate on sugar $kgCOD.kgCOD^{-1}$
$f_{ac,su}$	Yield of acetate on sugars $kgCOD.kgCOD^{-1}$

$f_{H2,su}$	Yield of hydrogen on sugars $kgCOD.kgCOD^{-1}$
$K_{s,su}$	Half saturation constant for sugar utilisers$kgCOD.m^{-3}$
$K_{s,c4}$	Half saturation constants of butyrate $kgCOD.m^{-3}$
$K_{s,pro}$	Half saturation constant for propionate utilisers$kgCOD.m^{-3}$
$K_{s,ac}$	Half saturation constant for acetate utilisers$kgCOD.m^{-3}$
$K_{s,H2}$	Half saturation constants of hydrogen $kgCOD.m^{-3}$
$k_{m,su}$	Maximum uptake rate for sucrose $kgCOD.m^{-3}$
$k_{m,c4}$	Maximum uptake rate for butyrate $kgCOD.m^{-3}$
$k_{m,pro}$	Maximum uptake rate for propionate utilisers$kgCOD.m^{-3}$
$k_{m,ac}$	Maximum uptake rate for acetate utilisers$kgCOD.m^{-3}$
$k_{m,H2}$	Maximum uptake rate for sucrose $kgCOD.m^{-3}$
ρ_{su}	Rate of uptake of sugar $kgCOD.m^{-3}$
ρ_{bu}	Rate of uptake of butyrate $kgCOD.m^{-3}$
ρ_{pro}	Rate of uptake of propionate $kgCOD.m^{-3}$
ρ_{ac}	Rate of uptake of acetate $kgCOD.m^{-3}$
ρ_{H2}	Rate of uptake of hydrogen $kgCOD.m^{-3}$
$pH_{UL,i}$	Upper pH limit for which no inhibition of reaction i
$pH_{LL,i}$	Lower pH limit for which complete inhibition of reaction i
$K_{I,NH3}$	Ammonia inhibition constant for acetate utilisers$kgCOD.m^{-3}$
$K_{r,p}$	Relative permeability (m^2)
$K_{i,p}$	Intrinsic permeability (m^2)
μ_p	Dynamic viscosity of each phase (liquid, gas)
ρ_i	Density of each phase (liquid, gas) (kg/m^3)
P_i	Pressure of each phase (liquid, gas) (Pa)
S_l	Liquid saturation.
S_r	Residual saturation
S_e	Effective saturation
α_g	Term the production of biogas
n	Porosity of the medium
V_i	Velocity of moving fluid (m/s)
$(\rho Cp)_f$	Volumetric heat capacity (J m^{-3} K^{-1})

General Introduction

"Nothing is born or perishes, but already existing things combine and then separate again" (Voilquin, 1964). This is how Anaxagoras of Clazomenae formulated in the 5th century BC, what would later become the principle of the law of mass conservation. This fundamental principle has long formed the basis of rational consumption. Thus for millennia, humankind, due to the limited techniques, has only carried out small withdrawals from nature and recycled, by any form of waste, thus controlling the cycle of matter. The industrial revolution which appeared at the end of the 18th century and the rapid evolution of techniques saw the emergence of a completely different form of behavior: the reckless exploitation of resources, whether renewable or not. Economic growth (corresponding to positive goods and services in the Mondial economy,) appeared as the main objective of the new society which has existed because of the industrial revolution which appeared at the end of the 18th century. By occupying the center of concerns and interests, it has become the impulsive as well as the driving force behind an increase in production and consumption. The incessant desire for this economic growth linked to an ever more pronounced world population growth which leads to maximizing efforts. energy needs as well as an ever-expanding consumption of natural resources. This impacts the planet earth resources and has the direct effect of producing waste and increasing greenhouse gases.

In the mid-1970s, it was estimated that the worldwide ecological footprint (this parameter measures human demand on nature) has overtaken the biological capacity of the earth. In 2007, the ecological footprint exceeded the earth's capacity by 50%, which means that it takes the earth a year and a half to reconstitute what we consume in one year.

And in 2016 the average ecological footprint was about 2,75 global hectares per person, Between the 1970s and 2000s, a third of the plant's resources were consumed (Hawken, et 2010) and pollution caused by anthropogenic activity accelerated sharply. From the 1970s, however, signals were launched on a global scale to warn of the harmful influence of human activity on the global balance of the planet and to alert of the emergence of a drastic reduction in emissions of greenhouse gases (GHG) due to waste generation and the use of fossil fuels (reports from GIEC of 1997, 2007). But the endeavors and efforts, taken from states of the world are still not enough and not yet significant to stem the phenomenon.

The overall reduction in pollution goes through a profound modification of individual behavior but also a reorganization of socio-economic systems. However, it also necessarily involves the implementation of alternative energy production and waste treatment techniques, the increasingly massive production of which is becoming an urgent global issue.

Now waste management has become one of the biggest issues for most countries in the world as well as a priority for our country's environmental policy. In the current context of sustainable development and the reduction of greenhouse gas emissions, the use of forest biomass and crop residues as a source of energy (heat, electricity) is becoming more and more popular as well more attractive. The current political climate will encourage the use of waste as a source of energy. The economic, environmental, and social arguments are in favor of this type of energy. Nowadays, waste has become one of the most competitive resources of renewable energy for heat and electricity production and is a widely available resource in Morocco.

Among the possible solutions for more sustainable management of waste, there are modes of biological treatments, in particular anaerobic digestion (AD), also called methanization.

This technique, which has been adapted over the last two centuries to an industrial scale, is based on a natural process of biological degradation of organic matter by a diverse population of microorganisms, in the absence of oxygen. It offers many advantages.

In addition to reducing the amount of waste by converting part of the organic matter into biogas, it allows, under controlled conditions, to recover this biogas, rich in methane, thus providing a solution suitable for the production of energy renewable as well as the reduction of greenhouse gases. It is for these reasons that AD technology is booming.

AD can play a strategic role in the development of waste management systems, since it is capable of treating almost all the biodegradable fractions and generally of the agricultural residues, animal waste, household waste, waste urban and industrial centers, etc. AD or methanization is a complex biochemical process carried out in the absence of oxygen and involving different microbial communities in the degradation and conversion of organic matter (OM) polymers into reduced end products, including high-value, biogas mainly composed of methane (55-75%) and carbon dioxide (30-45%).

Batstone (2002) presented with the publication of the ADM1 a general basic concept for modeling and simulation of anaerobic degradation processes. This model is intended as a common basis for the further development and application of mathematical models in various areas of anaerobic technology. This model is also appropriate as a starting point for use on agricultural substrates for biogas production, but there are special requirements and thus the need for model adaptation.

This work revolves around two main axes:

The development and application of biological models, suitable for AD technology.

A hydro-thermo-biological digital coupling model (mathematical model coupling).

The main focus of this thesis is the numerical modeling of AD processes in agricultural biogas plants, especially maize residues in Moroccan country which has an abundant percent of waste more than other cereal, whereas people use it only for combustion or to feed animals in a critical period of the year when there’s a lack of grasses. For this purpose, the widely recognized AD model No.1 (ADM1) has been utilized together with corresponding simulation software using FORTRAN. In the context of a research project dealing with the development of novel concepts of agricultural residues strategy followed by most developed countries. As well, the kingdom of Morocco launched in 2008 “the green plan” for the purpose of making agriculture as the main engine of economic growth. For the aim of the establishment of biogas plants in some future research, different aspects are taken into consideration during the investigation and simulation including corresponding modifications and adjustments of the mathematical model. This was inserted by laboratory experiments from other studies, and the data gained there was used for calibration and validation of the numerical models to fit the type of substrate used for the study.

The thesis is organized into four chapters, in addition to an introduction and general conclusion and perspective, in the first chapter, we constitute a bibliographical synthesis titled state of art, recalling the different types of organic waste that can be recovered by the AD process. As well, the history of its implementation from the past until the era of big industries, then some environmental interests of this technique. Also, an explanation of the different stages of the biochemical process of AD, namely hydrolysis, acidogenesis, acetogenesis, and finally methanogenesis, this later carried out with the bacterial populations which are involved in converting organic matter into biogas. Likewise, the key role of some important parameters that can influence the phenomenon of AD as well as the type of reactors and the alimentation method. Other subheadings of some relevant models from the literature of AD. Finally, we put statistics of some crops in the last subheading of this chapter in order to show the importance of agricultural residues for the production of energy.

In the second chapter, we develop the model called ADM1, by which we simulate the AD model for the production of methane gas, The ADM1 model used here for an adaptation to suit the agricultural field this latter comes from the field of wastewater treatment and is therefore designed according to the prevailing conditions in this area.

In the third chapter, we present the mathematical formulation of fluids (liquid and gas) and gas transfer. This chapter will be devoted to the second axis of this work: the modeling of the AD process. First, we present the development of a simple biological model, suitable for AD. Showing the effects of the stoichiometric and kinetic parameters such as half-saturation of Acetate, as well as the Monod constant of the main substrate. The kinetics of degradation of solid waste was based on mass conservation law, and the mathematical equations of gas transfer have been represented by arrhenius' law.

In the fourth chapter, we represent the numerical methods used with the discretization that we have chosen to solve the differential equations of mass transfer. The methods of the finite volume method and Runge Kutta were used to resolve the mathematical models of anaerobic digestion as well the heat transfer in the porous media.

In the fifth chapter, we present the analysis and interpretation of the results obtained for each case study, showing the effects of the key parameters that may strongly influence the production of methane gas.

At the end of this manuscript, we conclude by a general conclusion in which we discuss the perspective of future research, followed by the references and the annexes.

CHAPTER 1

STATE OF ART

1. Methanization

1.1. General principles of anaerobic digestion

Methanization called also anaerobic digestion which is a natural process that happens to organic matter, in the absence of oxygen, by a set of microbial flora. This biological process forms a stabilized and hygienized digestion residue, called digestate, as well as biogas which has a variable composition containing:

- Between 50 to 80% of methane CH_4.
- Between 30 to 50% of carbon dioxide CO_2.
- Saturated water H_2O.
- Some traces of NH_3, H_2S, N_2, CO.

Anaerobic digestion can be practiced in virtually all organic compounds natural and even some synthetic origin.

This biological degradation implies a specialized and diversified microflora that requires specific and adapted bio-physicochemical conditions, like all biological reactions, the reactions involved in the anaerobic degradation are carried out in the presence of water, that is to say in an aqueous medium (Moletta et Cansell, 2003).

Anaerobic digestion (AD) undergoes organic matter biodegradation in a complex biological process which takes four main steps: hydrolysis, acidogenesis, acetogenesis and methanogenesis as shown in *Figure 1*. each step of the degradation of the organic matter requires the activity of its specific group of microorganisms (Appels et al., 2008; Chandra et al., 2012; Kangle et al., 2012; Madsen et al., 2011):

Hydrolysis: this process occurs with hydrolytic microorganisms converting high molecular weight compounds and insoluble organic substrates such as carbohydrates, proteins, and lipids into smaller molecular materials and soluble organic substrates as sugars, amino acids and fatty acids (Appels et al., 2008).

Acidogenesis: this process occurs after hydrolysis where acidogenic microorganisms convert small molecular materials into volatile fatty acids VFAs (e.g., acetic, propionic, and butyric) along with the generation of carbon dioxide CO_2, hydrogen H_2, ammonia NH_3, ammonium NH4 (Appels et al., 2008).

Acetogenesis: this process occurs after acidogenesis where acetogenic bacteria convert organic acids VFAs into acetic acid along with H_2, CO_2 (Appels et al., 2008).The mixture of CO_2/ H_2 is transformed into acetate through homoacetogenesis (Monlau et al., 2013). Biodegradation process in anaerobic digestion.

Methanogenesis: which is the final process, this latter uses methanogenic archaea (mostly methanobacteriales and methanosarcinales) to convert acetic acid, H_2, CO_2 into methane CH_4 and carbon dioxide CO_2 (Appels et al., 2008; Guo et al., 2015; Madsen et al., 2011; Yu et al., 2014a). The mixture of CO_2/H_2 is transformed by hydrogenophilic methanogens into methane while acetate is converted into by acetoclastic methanogens (Monlau et al., 2013).

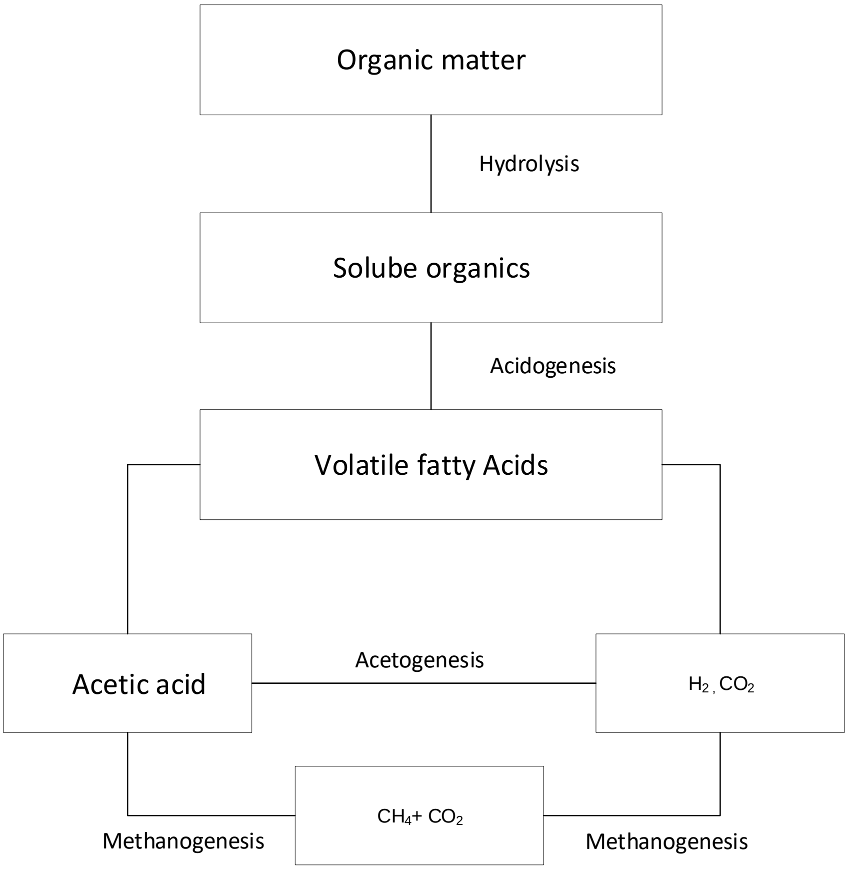

Figure 1: Biodegradation process in anaerobic digestion (Appels et al., 2008)

1.2. History and use of anaerobic digestion

The history of anaerobic digestion began in 1682 with Robert Boyle and Denis Papin both discovered that the decomposition of dead animals and plants produced a gas (Ranalli, 2007). In 1776, Alessandro Volta described “the flammable air of marshes, an air that burns very slowly with a beautiful blue flame” and highlighted the consequences of a complex set of chemical reactions on organic matter in poor environments of oxygen. Between 1804 and 1810 Dalton Henry and Davy have discovered the chemical composition of methane and claimed that the gas was similar to the swamp gas discovered by Volta. In 1884, Gayon, Student of Pasteur, produced 100 liters of methane per m3 of manure by fermentation at a temperature of 35 C. He also highlighted the ability of this gas to produce heat and light.

Figure 2: Engraving present Volta collecting methane in the marshes of Angera (Lombardy, Italy) by Ferry.

Anaerobic digestion is a complex phenomenon that occurs spontaneously in natural ecosystems, where organic matter is present in an anaerobic environment, such as marshes, lakes, rice paddies, lacustrine and marine sediments, soil, mammalian gut, the intestinal tract of certain termites, etc. (Servant, 1999; C Rouland, 1994).

Nowadays, in a global context where the demand for energy is increasing, the climate change is proven the necessity of sustainable development approaches, anaerobic digestion is a wise choice to answer these problems because it has several advantages (ADEME, 2015):
The production of renewable energy.
The production of a digestate with an agronomic value.
The reduction of greenhouse gases (GHG) by direct capture of methane emitted from organic waste or by substitution of biogas by fossil energy, and digestate to chemical mineral fertilizers.
The reduction of the quantity of organic waste, and in particular those which cannot be recovered by a composting system because they are too wet (grasses).

1.3. Anaerobic digestion industries progress throughout the world

Since May 31, 2011, biogas project holders must submit an identification file to ADEME before the application for connection to the public electricity grid. This initiative helps to monitor and facilitates the identification of projects and their installation. As of July 1, 2013, there are 242 projects built or under construction that are listed, for a total electrical power of 1,026 GW, all sectors combined (ADEME, 2013a). Agricultural biogas alone represents 58% of all known plants (*Figure 3*).

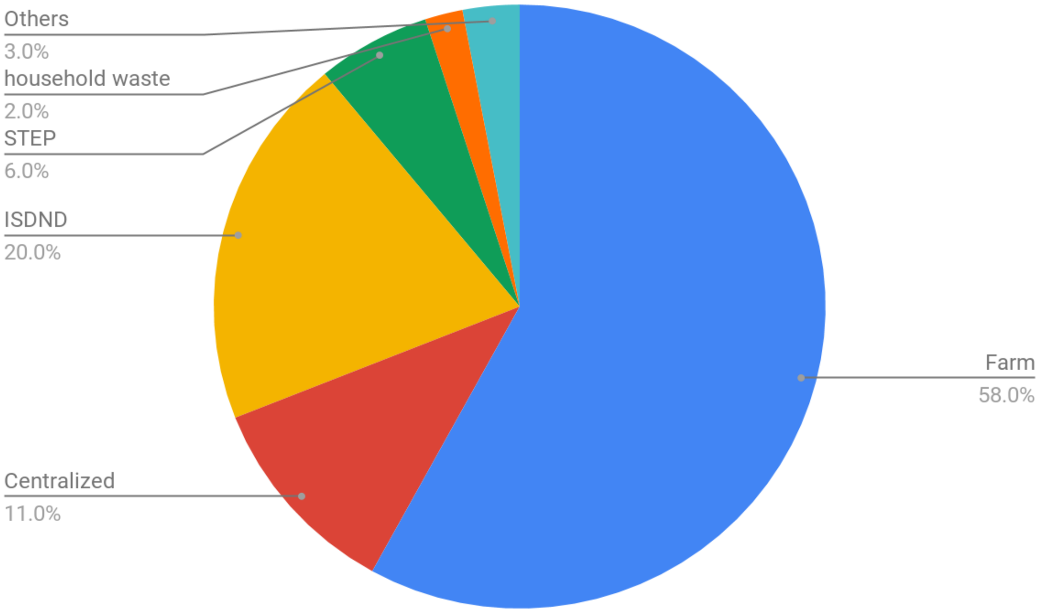

Figure 3: Distribution by sector of methanization units installed (ADEME, 2013)

Successive regulations, setting the purchase price for electricity produced by anaerobic digestion units, have led to the sustained development of the sector during the last decade. Thus, between 2010 and 2014, the number of "on-farm" biogas units increased fivefold from 31 to 166 plants in France (*Figure 4*).

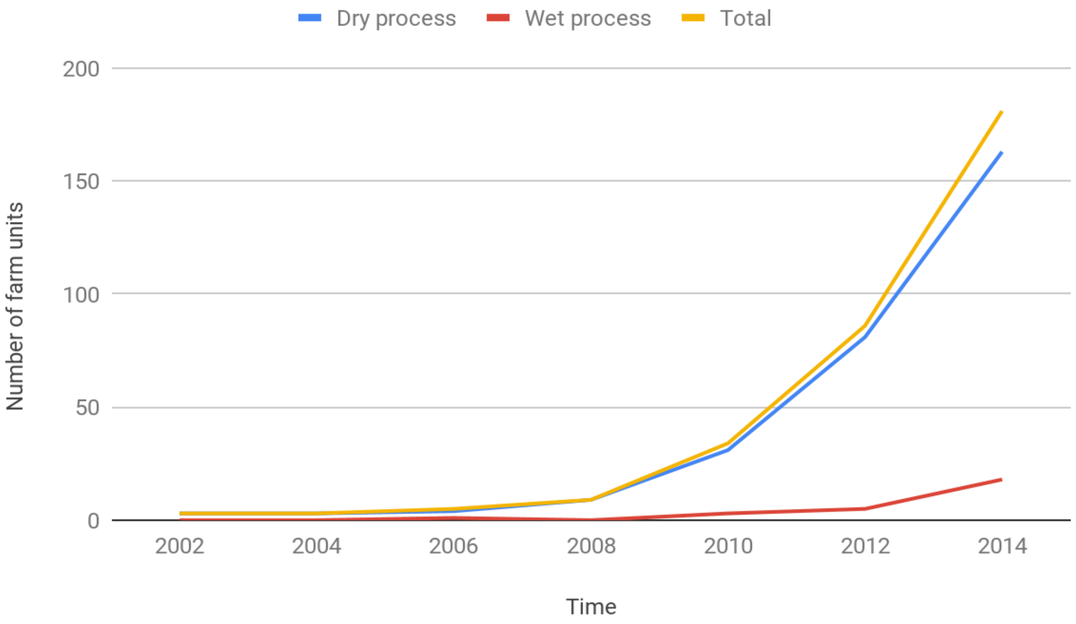

Figure 4: Evolution of the number of anaerobic digestion units from 2002 to 2014 by Sinoe with the

partnership of Irstea

This number, however, progresses at two speeds depending on the type of process used: liquid/ wet or solid/dry. This choice of the implementation of one or the other method is governed by the MS level of the substrates to be valorized. Substrates with an MS level greater than 15% (kg/kg) will be recovered in the dry process, and vice versa (De Baere 2000; Mata-Alvarez et al., 2000; Weiland, 2010). The *Figure 4* shows that wet anaerobic digestion is highly developed, with 149 projects registered at the end of 2014. On the contrary, only 17 solid-state facilities are listed on the same date.

1.4. The environmental interest of anaerobic digestion

Biological treatments are exclusively applicable to the biodegradable part of the waste deposits. Their application can be undertaken on a very broad variety of organic matrices. These biological treatments have various advantages. They allow:

To reduce the organic load of the waste (that is to say, the quantity of OM per unit mass) and thus to stabilize the mass of the waste.

To hygienize the matrix, that is to say, to reduce the quantity of pathogenic germs present in the waste.

To deodorize the environments.

To more easily dry the masses and thus treating them to burn them.

To spread (under certain conditions) the bio-treated products and thus to return directly to the soil part of the matter which has been removed from it.

To avoid certain nuisances associated with the management of landfill sites (generation of biogas, leachates, odors, etc…).

The issues related to biological treatment are multiple, whether in the short, medium, or long term. In the short term, the biological treatment makes it easier for organizations to manage waste that has been stabilized and reduced in mass (storage, transport, etc.) as well as an increased facility for drying it for incineration. In the average term, it provides simple and more reliable management of storage facilities. Finally, in the long term, the biological treatment makes it possible to return to the ground a part of the matter which has been subtracted from it. This is not insignificant given that, due to hundreds of years of intensive farming, the biological quality of agricultural soil deteriorates significantly.

2. The process of anaerobic digestion

2.1. The biochemical process of anaerobic digestion

2.1.1. Hydrolysis

Hydrolysis is the first of the four main biochemical processes of the methanization during which the biopolymers (proteins, lipids, carbohydrates) are hydrolyzed into water-soluble monomers and oligomers with extracellular enzymes excreted by microorganisms (Goel et al., 1998;

Sanders et al., 2000; Zhang et al., 2007). During this stage, the biopolymers will be transformed into their elementary constituent molecules. Thus, the hydrolysis products are different depending on the hydrolyzed substrate.

Cellulose or hemicellulose, carbohydrates are converted to (glucose, galactose, fructose) which are types of monosaccharides (Tong et al., 1990). Despite this, cellulose is highly resistant to biodegradation and hydrolysis because of its attachment to other biomass constituents such as hemicellulose or lignin (Peres et al., 1992) and because of its three-dimensional structure. Lignin is partially hydrolyzable to various aromatic compounds that may themselves be used by some bacteria but is considered to be virtually non-biodegradable under anaerobic conditions (Peres et al., 1992).

Proteins are converted to amino acids (Batstone et al., 2002) as well as polypeptides and ammoniums (Sanders, 2001).

Lipids are dissociated mainly in long-chain free fatty acids and glycerol (Batstone et al., 2002; Cirne et al., 2007).

The hydrolysis phase of lignocellulosic biomass is often considered to be the limiting step in anaerobic digestion (Vavilin, 1996; Batstone et al., 2002; Zhang et al., 2007; Myint et al., 2007).

2.1.2. Acidogenesis

Acidogenesis is the second step in the process of converting organic matter. It converts the products of the hydrolysis step into volatile fatty acids (VFAs), carbon dioxide, and hydrogen by an intracellular action of acidogenic bacteria. This biological reaction produces organic acids without acceptors or organic electron donors (Pavlostathis and Giraldo-Gomez, 1991). The degradation of monosaccharides, for example, may offer several degradation pathways as illustrated by three subsequent reactions (Batstone et al., 2002):

Table 1:

Table 1: Examples of glucose fermentation products (Batstone et al., 2002)

Products	Reaction
Acetate	$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COOH + 2CO_2 + 4H_2$
Propionate+Acetate	$3C_6H_{12}O_6 \rightarrow 4CH_3CH2COOH + 2CH_3COOH + 2CO_2 + 2H2O$
Butyrate	$C_6H_{12}O_6 \rightarrow CH_3CH_2CH_2COOH + 2CO_2 + 2H_2$
Lactate	$C_6H_{12}O_6 \rightarrow 2CH_3CHOHCOOH$
Ethanol	$C_6H_{12}O_6 \rightarrow 2CH_3CH_2OH + 2CO_2$

The degradation of sugars can nevertheless lead to the formation of other compounds such as lactate or alcohols, especially at low pH (a rare case in anaerobic digestion).

The flora responsible for hydrolysis and acidogenesis consists of facultative anaerobic bacteria, which develop relatively quickly (doubling time is a few hours) and tolerate relatively acidic pH up to pH 5 (Bayard and Goudron, 2011). They are also less specific to the substrate than methanogens (Yu et al., 2004).

The acids formed during the acidogenesis and hydrolysis phase of the lipids will then undergo another transformation step, the acetogenesis phase.

1.3. Acetogenesis

The acetogenesis step is the biochemical step of acetate formation from the hydrolysis and acidogenesis products (see *Figure 1*). This conversion can take place following two metabolic pathways with bacteria consuming either AGV or CO_2 and hydrogen (Batstone et al., 2002).
Acetogenic bacteria are strict anaerobes, very sensitive to pH, and have very slow growth (Zinder, 1993). The metabolic pathway of acetate formation from longer acids chains is β-oxidation. In contrast to the reactions that come into play in acidogenesis, microorganisms that oxidize organic acids necessarily require electrons, in this case, hydrogen (Pavlostathis and Giraldo-Gomez, 1991; Batstone et al., 2002). Those biochemical reactions, therefore, form hydrogen. The bacteria that convert AGVs to acetate, hydrogen, and CO_2 are called “hydrogen producers” (Malta-Alvarez, 2003). However, these reactions are thermodynamically unfavorable, as shown in *Table 2* and can, therefore, occur only with a very low partial pressure of H_2, and to a lesser extent at low product concentrations (Batstone et al., 2002; Siriwongrungson et al., 2007). It is, therefore, necessary to consume hydrogen so that its partial pressure decreases, and the β-oxidation reaction of AGV is thermodynamically possible.
This consumption of hydrogen is carried out by two metabolic pathways, one of which is the second metabolic pathway of acetogenesis, called homoacetogenesis, the other is hydrogen-plastic methanogenesis (see next paragraph). There is, therefore, a compulsory association between the species producing the hydrogen and those which consume it; this is called a syntrophic relationship (Schink, 1997; Mata-Alvarez, 2003; Huilinir et al., 2008; Nie et al., 2008).

Table 2: Thermodynamic reactions of Beta-oxidation of acids by microorganisms

Substrate	Reaction	ΔG^o	$\Delta G'$
Propionate	$CH_3CH_2COOH + 2H_2O \rightarrow CH_3COOH + 3H_2 + CO_2$	0.68	-0.13
Butyrate	$CH_3CH_2CH_2COOH + 2H_2O \rightarrow 2CH_3COOH + 2H_2$	0.3	-0.16
Palmitate	$CH_3(CH_2)_{14}COOH + 14H_2O \rightarrow 8CH_3COOH + 14H_2$	0.55	-0.16

ΔG’ is calculated at 298 K, pH=7, hydrogen partial pressure of 1x10-5 bar, and concentrations of organic acids of 1mmol.L^{-1}.
The formation of acetate from hydrogen and CO_2, called Homoacetogenesis is also a metabolic pathway present in the process of anaerobic digestion. It occurs by reduction of CO_2 according to the following reaction:

$$4H_2 + 2CO_2 \rightarrow CH_3COOH + 2H_2O$$

This metabolic pathway is often associated with anaerobic digestion taking place in psychrophilic conditions since homoacetogenesis are more apt to adapt to low temperatures compared to hydrogenotrophic methanogens (Kotsyurbenko et al., 2001; Nozhevnikova et al., 2003). Studies have suggested that homoacetogenesis cannot compete with methanogenesis in thermophilic and mesophilic regimes since the latter generates much more energy (Ahring and Westermann, 1987; Conrad and Klose, 1999; Batstone et al., 2002).

2.1.4. Methanogenesis

Methanogenesis is the last step in the anaerobic conversion process. This biochemical step can take place in two metabolic pathways: acetoclastic methanogenesis and hydrogenoclastic methanogenesis. This degradation process is carried out by strict anaerobic microorganisms called archaea. They are part of a specific group, the archaebacteria, which is separated from the reign of prokaryotic bacteria by metabolic characteristics as well as a particular membrane structure. The microorganisms responsible for this degradation step are characterized by slow development and high pH sensitivity (Bayard and Gourdon, 2001).

Acetoclast methanogens use acetate as a substrate according to the following overall reaction:

$$CH_3COOH \rightarrow CH_4 + CO_2$$

This metabolic pathway is responsible for 65% to 75% of the methane produced (Pavlostahis and Giraldo-Gomez, 1991).

Hydrogenotrophic methanogens reduce carbon dioxide with dihydrogen according to the following reaction:

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

This pathway is essential for the proper functioning of the whole biochemical process of anaerobic digestion because it allows us to maintain a low hydrogen pressure, essential for the acetogenesis phase to take place, as mentioned above. If this metabolic pathway is unbalanced, acetate formation by acetogenesis is slowed down, resulting in an accumulation of other VFAs.

2.2. Factors affecting anaerobic digestion

2.2.1. Temperature

Temperature is an important influence factor for anaerobic digestion. Conventionally, three temperature ranges are used in anaerobic digestion: psychrophilic (4-15 °C), mesophilic (20-40 °C) and thermophilic (45-70 °C) (Batstone et al., 2002). In each of these ranges, the bacterial floras that develop are different. Although the methanization reactors can work at operating temperatures situated within these domains, the two optimum temperatures conventionally used are 35 °C and 55 °C (mesophilic and thermophilic modes, respectively) with a decrease in activity bacterial around 45 °C. This phenomenon may be due to the effect of methanogenic bacteria that seem to have optimal temperatures consistent with the ranges mentioned. The *Figure 5* illustrates how the growth of the different groups of methanogens is dependent on the temperature according to the Arrhenius law up to the maximum (optimum), followed by a rapid fall.

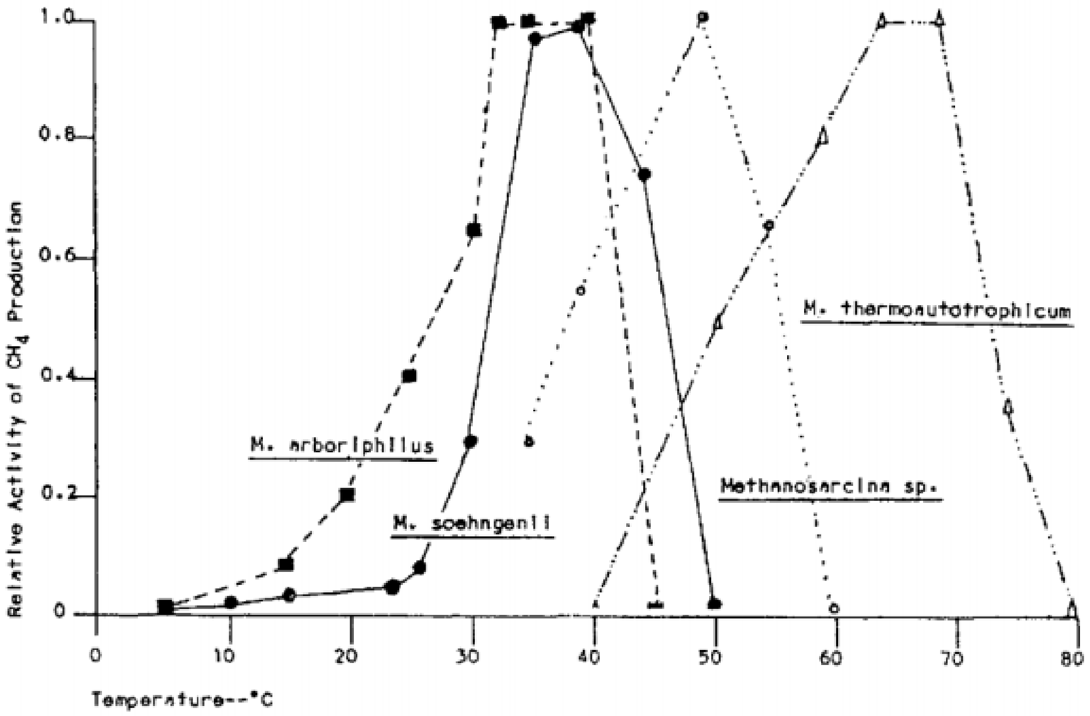

Figure 5: Growth rate of methanogens as a function of temperature (Marchaim, 1992).

In general, temperature affects 5 axis biochemical reactions (Batstone et al., 2002):

The increase in temperature induces an increase in degradation rates according to the Arrhenius law.

The increase in temperature above the optimum (>40 °C in mesophilic and > 65 °C in thermophilic) induces a decrease in degradation rate.

The increase in temperature (above the optimum) induces a decrease in yields due to an increase in the energy required for cell renewal and maintenance.

The temperature variation induces a modification of metabolic pathways and yields due to variations in thermodynamic conditions and bacterial populations, as we have seen for homoacetogenesis.

The increase of the temperature induces the increase of the mortality rate of the bacteria because of the phenomena of cell lysis and modified cell maintenance.

The temperature also influences the enzymatic activity which has the effect of modifying the rate of hydrolysis according to Arrhenius's law (Veeken and Hamelers, 1999; Mata-Alvarez, 2003).

The temperature also affects the physicochemical reactions of environments such as:

- The equilibriums of the chemical species present in the digestion media: ammoniacal nitrogen, sulfides, AGV by its action on the acid-base equilibria and oxide-reducers
- The liquid/gas equilibrium.
- The dissolution of solids.

The temperature, therefore, has a considerable influence on the physicochemical and biochemical processes of anaerobic digestion and optimal temperature conditions, especially for biochemical degradation processes, are at fairly high values (35 °C mesophilic and 55 °C thermophilic). However, the reactions involved in anaerobic degradation processes are slightly exothermic and therefore do not create much heat. It is, therefore, necessary to bring this heat to the reactors in order to obtain these ideal conditions. In industrial reactors, a change in temperature (e.g. failure of heating systems) will induce a reversible decline in methane production.

On the other hand, repeated temperature variations between different operating ranges (mesophilic and thermophilic) will lead to repeated modifications of the microbial communities as well to reaction metabolisms, inducing much more complex problems and the system will not be effective (Batstone et al., 2002). It is still important for industrial digesters to avoid even small variations in temperature that can affect the functioning of microorganisms and therefore the process in general (Zinder et al., 1984).

2.2.2. pH and alkalinity

pH plays a major role in the biochemical and Physico-chemical functioning of anaerobic digestion media. On the other hand, it will be able to alter the functioning of certain microorganisms, otherwise, it will influence the chemical equilibrium.

Although pH is a very difficult parameter to evaluate due to the complexity of the phenomena and species involved, it can be controlled by taking into account only a few chemical species (Mata-Alvarez, 2003): bicarbonates, AGVs as well as ammonium ions.

These species play a buffer role in the digestion media and each of these predominates species in particular pH ranges, ranging from 5.5 to 8. The ammonia/ ammonium pair predominates in high pH values, the couple bicarbonate-carbon dioxide in the mean values (neutral) whereas couples involving couples “AGVH-AVG” predominates in low pH values.

In addition to these buffers, biochemistry is also influenced by pH. Each microorganism has a pH range in which they develop optimally. In general, this optimum in pH ranges close to neutrality. But this consideration is only very general and the optimal pH ranges are variable for each type of microorganisms and even for the types of substrates that are treated.

Hydrolytic and acidogenic bacteria are not significantly affected by pH variations, which is not the case with acetogenic and methanogenic bacteria that do not tolerate excessive pH changes (Bayard and Gourdon, 2001). Despite this, hydrolytic activity is sensitive to pH changes (Veeken et al., 2000).

It has been shown that degrees of inhibitions of biochemical processes are closely related to the undissociated forms of the acids present in the media (Fukuzaki et al., 1990, Van lier et al., 1993). These undissociated forms, the amount of which depends on the pH of the media, diffuse more easily through the cell walls, causing internal pH drops in the bacteria. The effects of AGV concentrations are discussed more specifically in the section “Volatile Fatty Acids (VFAs)”.

Through similar phenomena, pH affects the growth of microorganisms through ammonia-ammonium equilibria. An increase in pH is responsible for an increase in the toxicity of

microorganisms due to the increase of the ammonia (NH_3) form in the milieu (Borja et al., 1996).
pH also plays an important role concerning liquid/gas equilibrium, especially for CO_2 which, being relatively soluble in water, reacts with water to form carbonic acid and this will affect the buffering capacity of the milieu.

Also, Alkalinity (m-Alk) measures the buffering capacity in an anaerobic digester and thus its ability to maintain a stable pH. This parameter, mainly related to the presence of dissolved CO_2 necessary for the growth of autotrophic bacteria, must be maintained above 2 g Eqt $CaCO_3.L^{-1}$ to prevent drastic drops in pH.

2.2.3. Volatile fatty acids (VFAs)

Volatile fatty acids (VFAs) are the most important intermediates of anaerobic digestion. Their accumulation in the digester indicates malfunctioning of the methanization, which is accompanied by a drop in pH and an increase in the hydrogen concentration that can lead to an inhibition of methanogenesis. For the good progress of an anaerobic digestion process, the concentration of volatile acids (TVA, Total Volatile Acidity) must be less than 2 g Eqt $CH_3COOH.L^{-1}$ to prevent inhibition of methanogenic bacteria (Yadvika et al., 2004). One of the criteria for confirming the stability of anaerobic bioreactors is the TVA/FAT ration which must be less than 0.4 (Callaghan et al., 2002).

2.2.4. Granulometry

The particle size of inputs affects the production of biogas (Kivaisi and Eliapenda, 1994). The granulometry should not be too large, otherwise, it would be difficult for the microorganisms to perform digestion, which decreases the production of gas.
It was found that in five different sizes (0.088, 0.4, 1.6, and 30 mm), the maximum volume of biogas was produced from substrates ranging in size from 0.088 to 0.4 mm (Sharma et al., 1988).

2.2.5. Agitation

Agitation promotes contact between the substrate and the microorganisms by facilitating the depolymerization and solubilization of the particles. Indeed, previous results have shown that good agitation promotes the acclimation of biomass and also limits various problems in digesters such as foaming, flotation, and super-saturation of certain gases that can form precipitates (CO_2) or act as inhibitors of reactions (H_2S and H_2) (Guillaume and Lendormi, 2015).

2.2.6. Carbon nitrogen (C\N) ration

The C/N ratio indicates the nutritive balance of substrates to be valorized. Carbon will be used by microorganisms as a source of energy and nitrogen is an essential nutrient for the development of these same microorganisms. If the amount of nitrogen is too low, the growth of microorganisms will be slowed down, the degradation of organic matter will be slowed down and the yield of methane will be reduced. In the opposite case, too high nitrogen concentration can lead to an accumulation of ammoniacal nitrogen, which is toxic for microorganisms.

Several authors agree to give an optimal ratio between 20 and 30 (Jha et al., 2011; Kothari et al., 2014; Wang et al., 2014). Hills (1979) advocates a ratio of 25 for the digestion of dairy cow manure. Other studies mention optimal C/N ratios of less than 20, suggesting that the optimal ratio depends on the digested substrate. The co-digestion of STEP sludge and onions, for example, is optimal for a C/N ratio of 15 (Romano and Zhang, 2008). That of household waste and cob corn has an optimal ratio between 15 and 18 (Kothari et al., 2014). In all cases, the nutrient balance, and in particular the C/N ratio can be adjusted by adding co-substrates (Callaghan et al., 1999; Zhang et al., 2008).

2.3. Alimentation

The factors related to the feeding of an anaerobic digester influence on several levels its operation. Indeed, depending on the organic loading rate (OLR) and the hydraulic retention time (HRT) applied to the digester, or the nature of the different substrates used, the production of biogas will be more or less quickly. Similarly, these different factors related to the aliment of the digester affect the amount of methane produced, the composition but also the risk of inhibition of microbial flora involved in the process of anaerobic digestion. The nutrients required by the microbial communities involved in the process are essential for their development because they allow the cell to synthesize the enzymes and cofactors necessary for biochemical and metabolic reactions (Anderson et al., 2003). To avoid any phenomenon of inhibition, it is therefore essential that the macro- and micronutrients (depending on their importance in the metabolism of microorganisms) be with sufficient quantities and available in the environment surrounding the microorganisms. However, an excess of some nutrients can be toxic to the microbial community and also lead to inhibitions (Gunnerson and Stuckey, 1986).

2.3.1. The nature of the substrates

The substrates used in bio-methanization mainly come from (1) agriculture, by the valorization of farm waste such as manure, refusal of food, waste of crops products such as energy plants (immature rye silage, maize, grass, sorghum), grain waste or straw and chaff; (2) agro-food industries, through the recovery of many wastes and co-products such as slaughterhouse waste, brewery grains, non-compliant vegetables and fruits, and rinsing water from machines and tools; (3) municipalities by the recovery mainly of wastewater and all types of organic waste such as lawn clippings, hedge trimmings, dead leaves or the remains of canteens.

2.3.2. Organic loading rate (OLR)

Under the action of the microbial complex, the degradation of the organic matter (OM) occurs continuously in a digester, until all the OM is consumed. The organic loading rate (OLR) defines the amount of substrate that can be incorporated, on a daily basis, for example, in the digester. This rate is an important parameter and must be adapted to microorganisms involved in the anaerobic digestion process. Indeed, the incorporation of a large amount of substrates in a digester where the microbial communities are unsuitable would lead to the rapid growth of the bacterial communities involved in the early stages of the anaerobic digestion process, because of their rapid generation time. As a result, a large amount of AGV from the degradation of the OM would be produced in the digester. This would lead to an inhibition of the development of methanogenic archaea, which cannot adapt to a high concentration of AGV and low pH values.

2.3.3. The hydraulic retention time (HRT)

The hydraulic retention time (HRT) is the time needed to replace the entire contents of the digester. It is calculated by dividing the total volume of the digester by the volume of the substrate introduced into it every day. The optimal HRT of a digester depends on the nature and composition of the substrates used to feed it, the digestion temperature, as well as the microbial community involved in the process (the type of microorganisms and density).

2.4. Types of reactors and operations

A lot of different types are used for agriculture biogas plants, one can distinguish between dry and wet processes (Laaber, 2007) and further between discontinuous and continuous processes (Bischofsberger et al., 2005). There are no typical plant types for a specific range of applications, each plant is planned individually (Laaber, 2007).

2.4.1. Discontinuous or batch mode

In the batch mode, the sealed reactors are initially filled with organic material to be treated and seeded with inoculum. The reaction proceeds without the exchange of material with the outside and continues until the depletion of the substrate to be degraded. At the end of the digestion, the reactor is drained and a new cycle can begin. This mode is generally used for determining the methanogenic potential of waste.

2.4.2. Continuous mode

Continuous mode operation is the most common on an industrial scale. The continuous reactors are continually supplied with a so-called “nominal” regime, which generally corresponds to a constant material flow rate. In parallel, an equal amount of digestate is removed from the reactor which will thus retain its useful volume. This technology is ideal for large installations. This operating mode is simple and generally adapted to the treatment of effluents heavily loaded with organic matter (agricultural waste, sludge urban…)

2.4.3. Semi-continuous mode

This mode of operation also called fed-batch or Sequencing Batch Reactor (SBR) is a hybrid model between continuous and discontinuous. It consists of applying, in a digester, cycles alternating filling, reaction, and emptying.

The advantage is to retain all or part of the microorganisms in the reactor for the next cycle. This model is well suited to small biogas plants.

• 3. Anaerobic digestion modeling

The modeling of the anaerobic digestion process represents here all the methods likely to describe the evolution, temporal or not, of the compounds coming into play in the metabolisms of anaerobic digestion.

3.1. Conversion of organic matter to methane

3.1.1. Chemical oxygen demand

During anaerobic digestion, the conversion of organic matter (OM) can be simplified according to the following equation (Tchaobanoglous et al., 1993):

$$OM + H_2O\ \mu \rightarrow\ n_{\mu} + \mathrm{OM}_{\text{recalcitrant}} + CO_2 + CH_4 + \text{gas}_{\text{various}}$$

Part of the organic matter (OM) is used by the microorganisms (μ) to synthesize new biomass (n_{μ}). It should be noted that on the fraction of converted organic matter, 10% by weight is found in the form of microbial biomass (the rest, therefore, in the form of biogas).

This number is comparable to that obtained by aerobic treatments, in which 50% of the degraded organic matter is converted into biomass (Moletta, 2015). The biogas formed consist of combustible methane (50% to 70%), carbon dioxide (25 to 45%), and various trace gases (NH_3, H_2S, CO, etc.).

The measurement of chemical oxygen demand (COD) is often used to characterize organic matter. The theoretical maximum production of methane is a quantity associated with COD. considering total degradation, the amount of biogas formed by anaerobic digestion of organic material (of the form $C_nH_aO_b$) can be determined theoretically, using the Buswell equation (Buswell and Meuller, 1952).

$$C_nH_a\,O_b + (n - \frac{a}{4} - \frac{b}{2})H_2O \rightarrow (\frac{n}{2} + \frac{a}{8} - \frac{b}{4})CH_4 + (\frac{n}{2} - \frac{a}{8} + \frac{b}{4})CO_2$$

This balance equation, to which are sometimes added “d” nitrogen atoms to the organic molecule and “dNH_3” to the products, has been balanced by considering a total conversion of the organic matter into CH_4 and CO_2 under anaerobic conditions, i.e. in the presence of H_2O only.

Using this balanced equation and knowing the elemental composition of the organic matter considered, it is, therefore, possible to estimate the theoretical maximum potential of biogas production.

Moreover, the COD is, by definition, the quantity of oxygen necessary for the oxidation of this same organic compound according to the formula:

$$C_n\, H_a O_b + (\, n + \tfrac{a}{4} - \tfrac{b}{2})O_2 \rightarrow n\, CO_2 + \tfrac{a}{2} H_2O$$

It should be noted that there is a proportionality between the quantity of methane produced by the anaerobic digestion of a compound and the quantity of oxygen necessary for its total oxidation:

$$\frac{n_{CH_4}}{n_{O_2}} = \frac{\frac{n}{2} + \frac{a}{8} - \frac{b}{4}}{n + \frac{a}{4} - \frac{b}{2}} = \frac{1}{2}$$

This proportionality makes it possible to define a theoretical maximum methane yield of 0.35 Nm^3.kg COD^{-1} (Moletta, 2015). This ratio is often used to establish operating budgets for biogas digesters.

3.1.2. Methanogenic potential and anaerobic biodegradability

The theoretical estimate of methane produced does not take into account the consumption of organic matter for microbial metabolism and the possibility of having some recalcitrant or non-bio-available compounds for degradation. For that, tests make it possible to determine the potential methanogenic of the organic matter (BMP, Biochemical Methane Potential), that is to say, the maximum quantity of methane that they are likely to produce.

Significant variability is sometimes observed in the literature for the BMP of the same substrate due in particular to the differences in experimental conditions and inoculum used (Angelidaki and Sanders 2004; De Vrieze et al., 2015; Raposo et al., 2012).

These tests are performed in batch mode and consist of following the production of biogas or methane of a substrate-inoculum mixture (source of anaerobic microorganisms) over time. The mixture is introduced into an airtight, placed under anaerobic conditions, and incubated at the desired temperature. The net value of methane production of the substrates is obtained by subtracting the endogenous production of the inoculum alone.

Many factors can influence the results of these tests, including substrate concentration, inoculum/ substrate ratio, the origin of the inoculum, and experimental monitoring device (Liu et al., 2009; al., 2015). The tests are continued until the production of biogas is stopped. However, the test times vary from 12 to 87 days depending on the laboratory with the majority of protocols taking place for 25 to 40 days (Raposo et al., 2011).

The methanogenic potential is calculated by dividing the volume of methane produced by the amount of COD injected (Nm^3 CH_4. kg COD^{-1}), under normal conditions of temperature and pressure (0 °C, 1,013 bar). The anaerobic biodegradability of the substrates (%) can also be determined by dividing the methanogenic potential by the maximum theoretical CH_4 yield of 0.35 Nm^3 CH_4. Kg COD^{-1} (Buffiere et al., 2006).

3.1.3. Chemical kinetics

The hydrolysis reaction of macromolecules is generally considered to be the reaction limiting the overall process of anaerobic biodegradation (Pavlostathis and Giraldo-Gomez, 1991). Thus, the methanogenic potential can be used to determine the overall hydrolysis constant k_h. in descriptive terms, this reaction step is typically simplified and reduced to first-order kinetics (Bilgili et al., 2009; Eastman and Fergurson, 1981). In this case, it will be possible to write the following equation:

$$V_{CH4}(t) = V_{CH4} \times [1 - exp(-k_h \times t)]$$

With V_{CH4} (t), the volume of methane produced over time ($Nm^3.kg\ COD_{initial}{}^{-1}$) and k_h, the hydrolysis constant (d^{-1}).

On the other hand, the modified Gompertz equation was used to analyze the cumulative productions of methane, and more particularly those with early latency phases (Lo et al., 2010). It was originally developed to analyze bacterial growth curves and was later modified to describe the cumulative production of methane in batch culture. It is expressed according to :

$$V_{CH_4}(t) = V_{CH_{4.max}} \times exp\left\{-exp\left[\frac{R_m \times e}{V_{CH_{4.max}}}(\lambda - 1) + 1\right]\right\}$$

With λ, the latency time (d); R_m, the maximum rate of methane production ($Nm^3.\ kg\ COD^{-1}.\ d^{-1}$), and e, the exponential of 1.

3.1.4. Main inhibitors

AGVs are the most commonly encountered inhibitors in digesters as mentioned previously. The toxic effect of long-chain fatty acids can also be reported during anaerobic digestion of lipids (Hwu et al., 1998). In the case of toxic inorganic compounds, there are several cations such as sodium (Na^+), potassium (K^+), heavy metals (Cu, Ni, Zn, Pb), ammonia (NH_3) and Hydrogen Sulphide (H_2S) (Moletta, 2015). These last two are often generated during the anaerobic digestion of high protein or sulfate waste and their effects have been widely studied. Reduced nitrogen, in ammoniacal form, becomes an inhibitor of methanisation beyond a few grams per liter (Hansen et al., 1998).

Hydrogen Sulphide is the product of the reduction of sulfate-reducing bacteria that compete with methanogenic Archaea for hydrogen consumption. This competition is governed by the COD / SO_4 ratio of the effluent. For a ration greater than 2.7, methanogenesis is preferred and when it is less than 1.7, the metabolism of sulfate-reducing bacteria will be favored (Choi and Rim, 1991). The presence of H_2S also leads to corrosion problems that require pretreatment of the biogas before use. On the other hand, organic compounds (phenols, organo-halogens, amides, amines, nitriles, ketones, fatty acids, etc.), disinfectants, antibiotics in livestock effluents and pesticides in crop residues, are all toxic compounds for the methanogenic microflora that will be irreversibly inhibited by their presence (Chen et al., 2008).

3.2. Relevant models proposed in the literature

3.2.1. Simplified model: kinetics of order 1

3.2.1.1. General case

In the case of anaerobic digestion, first-order kinetics is often used, for the hydrolysis step for example.

With the modeling of order 1, the decay of the concentration of a substrate is simulated as being exponential. Applied to anaerobic digestion, the kinetic approach allows describing the evolution of the concentration of organic matter over time, directly proportional to the amount of methane formed.

3.2.1.2. Hydrolysis of organic matter in anaerobic digestion

The hydrolysis step aims to solubilize the substrates. This step is carried out thanks to extracellular enzymes secreted by certain bacteria. It is therefore not a biological stage strictly speaking because there is no metabolism. This step is often considered as the limiting step of anaerobic digestion.

First-order kinetics have been shown to adequately simulate this biochemical step (Pavlostathis and Giraldo-Gomez, 1991; Mata-Alvarez et al., 2000; Batstone et al., 2002; Vavilin et al., 2002; Mora-Naranjo et al., 2004). This kinetic of the first order is of the following type:

$$\frac{dX}{dt} = -k_h.X$$

Where X is the concentration of hydrolyzable material [M], $[L]^{-3,}$ and k_h is the hydrolysis constant $[T]^{-1}$.

This first-order kinetics, however, reflects the cumulative effect of a set of processes (Veeken et al., 2000; Batstone et al., 2002; Vavilin et al., 2002), and the rate of hydrolysis depends on the amount of material that remains to be hydrolyzed, the extracellular enzymes being in excess relative to the substrate.

The hydrolysis constants are different for each substrate. The determination of these constants is carried out using specific experiments in which the consumption of substrate or the production of AGV for example is measured.

Table 3 gives the hydrolysis constants reported by the literature. As we see, there is great variability of these kinetic constants, even for a similar substrate, thus underlining the importance of certain factors (temperature, pH, etc.) that are not always the same in the tests carried out.

Table 3: Hydrolysis constant of OM cited in the literature.

Substrate	Hydrolysis constant	Temperature	Reference

Carbohydrates	0.041-0.13	30-40	Gujer & Zehnder, 1983 extract of (Batstone et al., 2002)
Lipides	0.04-0.08		
Protein	0.02-0.03		
Cellulose	0.02-2.88	35-37	(Pavlostathis & Giraldo-Gomez 1991)
Lipides	0.3-0.7		
Protein	0.04-1.12		
Biowaste	0.08-0.26	30	(Veeken & Hamelers, 1991)
Readily biodegradable	0.2-0.7	NR	(Mora-Naranjo et al., 2004)
Hardly biodegradable	0.00002-0.7		

3.2.2. Bacterial kinetics

3.2.2.1. General case

The steps of acidogenesis, acetogenesis, and methanogenesis are metabolic steps in which the substrates are consumed and transformed by bacteria. These biological kinetics are described by three phenomena: substrate consumption, bacterial growth, and bacterial death (decay).
Bacterial growth is represented by the following dynamic equation:

$$\frac{dB}{dt} = \left(\mu - k_d \right) B \qquad \text{Eqt. 1}$$

In which B is the hydrolyzable substrate concentration $[M].[L]^{-3}$, μ the growth rate $[T]^{-1}$, and k_d the first-order decay rate$[T]^{-1}$.
The kinetics of growth is associated with the kinetics of using the substrate:

$$\frac{dS}{dt} = -\frac{dB/dt}{Y} \qquad \text{Eqt. 2}$$

Where S is the substrate concentration $[M].[L]^{-3}$ and Y is the biomass yield (i.e., the fraction of substrate converted to biomass by cell metabolism).

The substrate can then become the factor limiting the growth of the microflora. To simulate this phenomenon, the model of Monod makes it possible to represent this rate of growth in many cases:

$$\mu = \mu_{max} \frac{[S]}{K_S + [S]} \qquad \textit{Eqt. 3}$$

Where μ_{max} is the maximum growth rate $[T]^{-1}$ and K_s is the half-saturation constant $[M].[L]^{-3}$, the substrate concentration when the growth rate is equal at half the maximum growth rate.

The combination of Equations 1,2 and 3 allows to express the variations of bacterial concentrations (Eqt 4) and substrate concentrations (Eqt 5) as follows:

$$\frac{dB}{dt} = \left(\frac{\mu_{max}.S}{K_S + S} - k_d \right).B = \left(\frac{Y.k_m.S}{Ks + S} - k_d \right).B \qquad \textit{Eqt. 4}$$

$$\frac{dS}{dt} = -\frac{1}{Y} \left(\frac{\mu_{max}.S}{K_S + S} - k_d \right).B = -\left(\frac{k_m.S}{Ks + S} - k_d \right).B \qquad \textit{Eqt. 5}$$

Where k_m represents the specific rate of Monod use for a given substrate $[T]^{-1}$.

These equations, therefore, make it possible to describe a biological transformation in which a substrate is transformed into degradation products using a microbial flora.

The variation of the product concentration of degradation (P) is obtained by the conservation of the material during the biochemical reaction of type:

$$-\frac{dS}{dt} = \frac{dB}{dt} + \frac{dP}{dt} \quad \rightarrow (\, Degraded\ subsbtrat = bacterial\ growth + reaction\ product\,)$$

$$\frac{dP}{dt} = -\frac{dS}{dt} - \frac{dB}{dt} \quad \rightarrow \quad \frac{dP}{dt} = \frac{1-Y}{Y} \left(\frac{\mu_{max}.S}{K_S + S} \right).B = (\,1 - Y)\,.\left(\frac{k_m.S}{Ks + S} \right).B \qquad \textit{Eqt. 6}$$

This system of three equations (Eqt 4,5 and 6) makes it possible to simulate a system comprising a substrate, microorganisms, and degradation products.

If we consider that the substrate is degraded into several reaction products (such as the degradation of propionate for example), product formation kinetics will then involve stoichiometric coefficients of the partition (η_i). The product concentration variation then becomes:

$$\frac{dP}{dt} = \sum_i \eta_i .(1 - Y) . \left(\frac{k_m .S}{K_S + S} \right) .B$$

These kinetics equations, applied to all of the substrates, intermediates, and products of the anaerobic degradation process, make it possible to model the biochemical phenomena involved in the degradation of organic matter. All models involving biological kinetics work in this way.

3.2.1.2. Modeling of inhibition phenomena

There are three different ways of modeling inhibition/toxicity phenomena: empirical laws, Monod laws with kinetic constant adjustment, and inhibition coefficients (Pavlostathis and Giraldo-Gomez, 1991).

In anaerobic digestion, the most commonly used method for biochemical processes is that of inhibition coefficients, although empirical type inhibitions are also used, in particular, to simulate the influence of pH.

Concerning reversible inhibitions, three types of expressions are used; competitive inhibitions; noncompetitive inhibitions, and incompetitive inhibitors (Pavlostathis and Giraldo-Gomez, 1991; Batstone et al., 2002).

Among these forms of reversible inhibitions, noncompetitive inhibition is the most frequently used for modeling in anaerobic digestion (Batstone et al., 2002) because it allows simple integration into the model of the effect of several inhibitors simultaneously under the following form:

$$\rho_j = \frac{k_m S}{K_S + S} X .I_1 .I_2 ...I_n$$

With $I_{i,}$ the functions of inhibitions used and ρj the rate of degradation of the compound j $[M].[L]^{-3}.[T]^{-1}$.

Some functions can also simulate inhibitions that occur when a compound (e.g. nitrogen) becomes limiting. This is the case of secondary substrate inhibitions.

Concerning pH-induced inhibitions, the models used often incorporate empirical functions that may take into account inhibitions only by low pH or inhibitions by high and low pH. *Table 4* illustrates the main forms of inhibitions used in the ADM1 model.

3.2.1.3. Modeling the pH of the medium

The calculation of the pH is carried out thanks to the taking into account of a set of three principal relations on the various chemical species of the medium:

- a global electroneutrality relation of the medium.

$$\sum \left[C^+ \right] - \sum \left[A^- \right] = 0$$

With $[C^+]$ the concentration of cations and $[A^-]$ the concentration of anions.

A relation on each of the acid /base pairs (HAc/Ac$^-$) according to which the total concentration [Ac $_{tot}$] of a compound is equal to the sum of the dissociated form [Ac$^-$] and the combined form [HAc].

$$[Ac_{tot}]=[HAc]+[Ac^{-}]$$

An acid/base equilibrium relationship involving the acidity constant (K$_a$) of the given pair.

$$K_a=\frac{[H^+].[Ac^-]}{[HAc]}$$

By coupling the last two relations, it is possible to know the concentration of free acid as a function of the total concentration of the element of the couple and the concentration of H$^+$ ions as follows:

$$[Ac^-]=\frac{K_a.[Ac_{tot}]}{K_a+[H^+]}$$

By applying this last relation to all the couples present in the digestion media and injecting it into the electroneutrality relation, we obtain an equation in which the only unknown is the concentration of H$^+$ ions (the total concentrations of each couple being given by the biological model explained above), and thus the pH of the medium via the relation:

$$pH=-log[S_{H+}]$$

Table 4: The principal form of inhibition used for the modeling of anaerobic digestion.

Description	Models	Used for
Non- competitive inhibition	$I=\frac{1}{1+\frac{S_I}{K_I}}$	hydrogen inhibition free ammonia inhibition
Empirical inhibition Low and Upper	$I=\frac{1+2\times10^{0.5(pH_{LL50}-pH_{UL50})}}{1+10^{(pH-pH_{UL50})}+10^{(pH_{LL50}-pH)}}$	pH inhibition when both high and low pH inhibition occur
Empirical inhibition Low	$I_{pH,i}=exp\left(-3\left(\frac{pH-pH_{UL,i}}{pH_{UL,i}-pH_{LL,i}}\right)^2\right)\ if\ pH < pH_{UL,i}$ $I_{pH,i}=1\ if\ pH>pH_{UL,i}\ with\ i=aa,ac\ and\ H_2$	pH inhibition when only low pH inhibition occurs
Competitive consummation	$I=\frac{1}{1+\frac{S_I}{S}}$	Competition of Valerate and Butyrate for C4

Substrate limitation	$I = \dfrac{1}{1 + \frac{K_I}{S_I}}$	All the biochemical processes

All the phenomena synthesized in this part allow us to set up a biological model capable of simulating the evolution of the chemical compounds involved in the anaerobic digestion process illustrated in *Figure 1*.

To complete the model, it is also possible to add additional relationships such as mass transfers between the different phases (solid, liquid, and gaseous), the effect of temperature or water content. These phenomena as well as their modeling will be explained further.

3.2.2. The complete model for anaerobic digestion: ADM1

The ADM1 model is a structural biological model that reflects the major mechanisms for converting complex organic substrates into biogas and degradation byproducts (Parker, 2005). The model coupled microbial kinetic equations with the formation/degradation equations of liquid and gaseous compounds by introducing inhibitory functions (Fezzani and Ben Cheikh, 2008). A total of 26 dynamic state variables (concentrations) are coupled to 19 kinetic biochemical processes, 3 kinetics of liquid-gas transfer as well as 8 implicit algebraic variables (Batstone et al., 2002) to describe the behavior of components. Soluble, particulate, and gaseous in a system considered perfectly homogenous. This model makes it possible to simulate the evolution of the compounds present in anaerobic digestion media, the evolution of pH and concentrations of microorganisms. The ADM1 model is a complete modeling model of anaerobic digestion processes developed for the simulation of diluted (wet) media.

• 4. Crops and residues

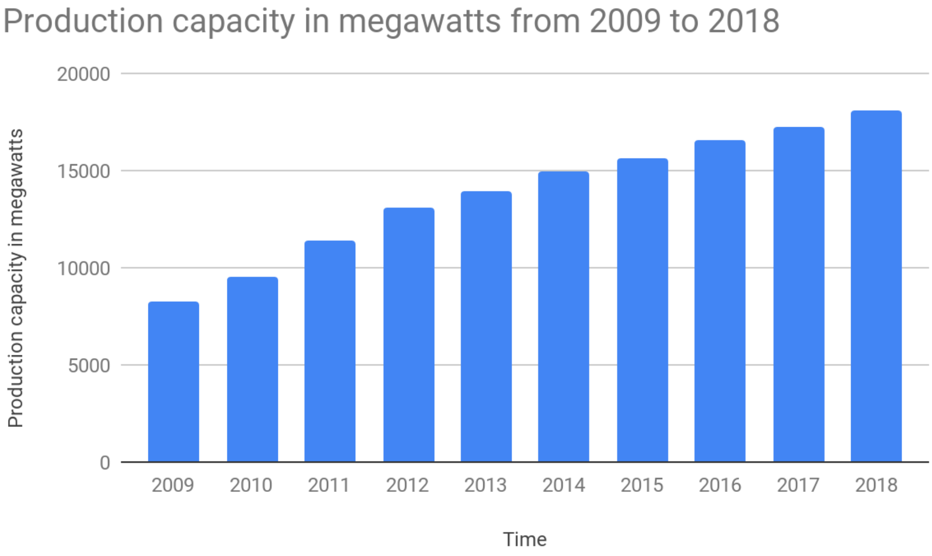

Figure 6: Installed capacity of biogas-derived energy worldwide from 2009 to 2018 by T. Wang, Aug 9, 2019

Agricultural activities inevitably generate waste which is more or less specific depending on the production sector. Some wastes pose risks to the environment (special wastes), others have significant recovery potential (compostable organic wastes, wood, biomass…)

Organic waste from crops is more and more frequently recycled as a fertilizer and soil improvers in vegetable fields.

As well as the need for energy leads the countries to adopt new policies for the production of green energies such as methane, electricity…

Agriculture is a very important economic sector in Morocco. It generates around 14% of gross domestic product (GDP), with significant variations (11 to 18%) depending on the precipitations during the year.

Its performance even conditions that of the entire economy: the country’s growth rate is strongly correlated with agricultural production. Agriculture also remains the country's largest provider of jobs, far ahead of other economic sectors, with 40% of the working population living in this sector.

4.1. Most relevant crops and residues

The *Figure 7* below shows the ten most produced crops worldwide in 2018, those crops are described by the average production from the year 1997, the highest production is taken by sugar cane and lowest production is for wheat. Those statistics are taken from the database of the Food and agriculture organization (FAO-2018).

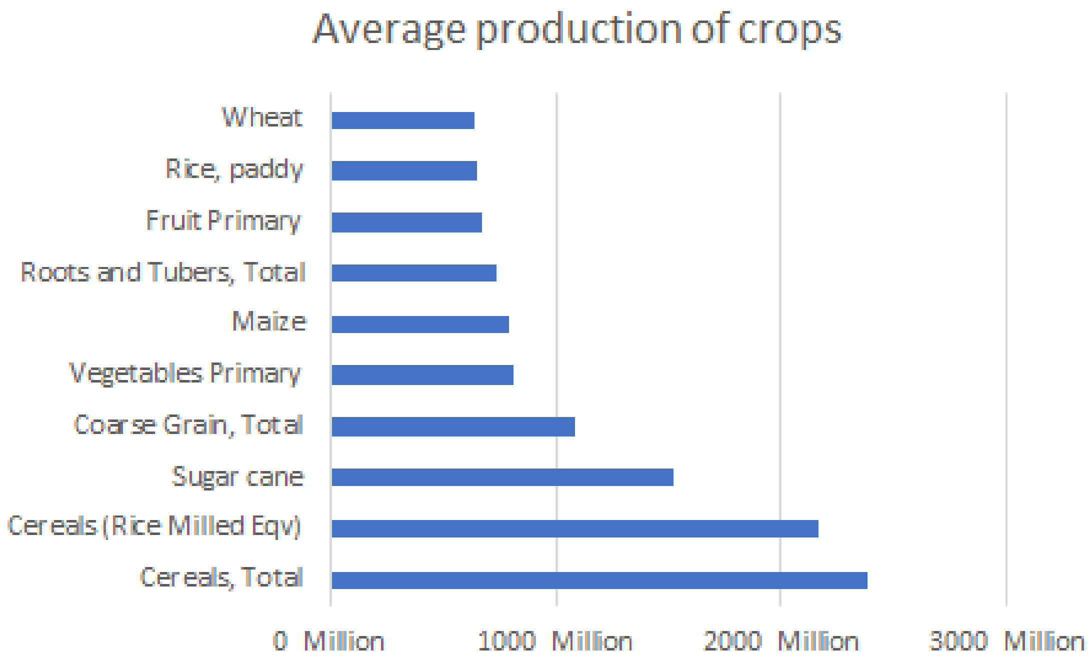

Figure 7: The average production of crops worldwide in 2018 (FAO-2020)

Crop residues are the aerial parts of plants not harvested and left on the ground in fields at the time of harvest, such as stems and stubble, leaves and pods for example.

The residues represent a significant amount of organic matter (OM), often greater than the harvested products such as maize. They can be valued in different ways: either recycled on-site to restore soil fertility, or removed from the fields as resources for other uses such as animal feed, soil amendment or fertilizer, energy production or industrial processing. In the first case, they can be buried as they are in the soil by cultivation or plowing, or after being burned.

Proper management of crop residues can improve the efficiency of irrigation and limit soil erosion. When used to feed livestock, residues can be recycled at least partially by spreading manure on cultivated plots.

These residues can be compared to waste from the first transformation of agricultural products into usable resources. This waste includes, in particular, leaves, seeds, cereal bran, rice hulls, bagasse, molasses, and roots.

The importance of crop residues is considerable when compared to the volumes harvested for the production of food for humans and livestock, or fiber. However, there are no official statistics on the volume of residues produced by country or worldwide, but only evaluations from studies concerning the management of agro-ecosystems, the potential energy of biomass, animal feed, or emissions of greenhouse gas. An assessment, based on the concept of harvest index, puts the global volume of residues in the 1990s at 3,75 billion tonnes of dry matter, for an average harvest index of 0.421, which means that residues of crops represent on average 58% of the phytomass produced by crops.

Table 5: Residue to grain ration (U.S.Department of Energy 2011)

Crop	Residue to grain ratio
Corn	1.0
Sorghum	1.0
Oat	2.0
Barley	1.5
Wheat	1.5

4.2. Corn cultivation

Maize or sweet corn (Zea mays saccharate Sturt) that belongs to the Poaceae family, it has a high nutritional value among the carbohydrates crops, it is used especially for food and feed and it is produced in the five continents. It originates from North America. The culture is unknown in Morocco although the product is imported from abroad (Spain) in cans.

While most grains favor planting in the fall or spring, corn (Zea mays) is grown in the summer. It requires minimum temperatures of 10 °C for its germination and 18 °C for its flowering.

Sweet corn is harvested between 80 to 120 days after sowing. The harvest is generally spread from the end of July to October. The harvest depends on several criteria: the precocity of the variety, watering, heat…

4.2.1. Availability and geography dispersion

The data taken from the minister of agriculture of Morocco are quite similar to the data released by the US Department of Agriculture (USDA).

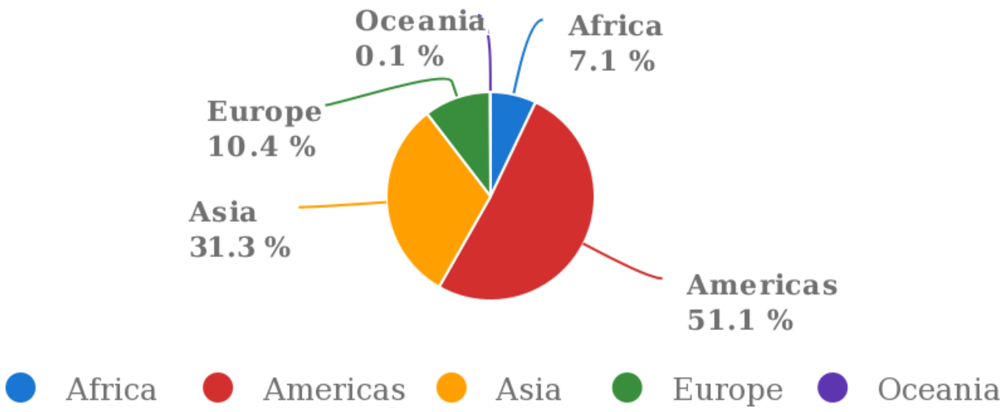

Figure 8: The average production share of maize by region (2017_2018) (FAO-2020)

The world corn production has risen sharply, from 150 million tons in 1950 to almost 840 million tons on average since the start of the 2010s. The main producers are the United States, China, and then practice on an equal footing, Brazil, and the European Union. France alone achieves about 25% of the production of the European Union.

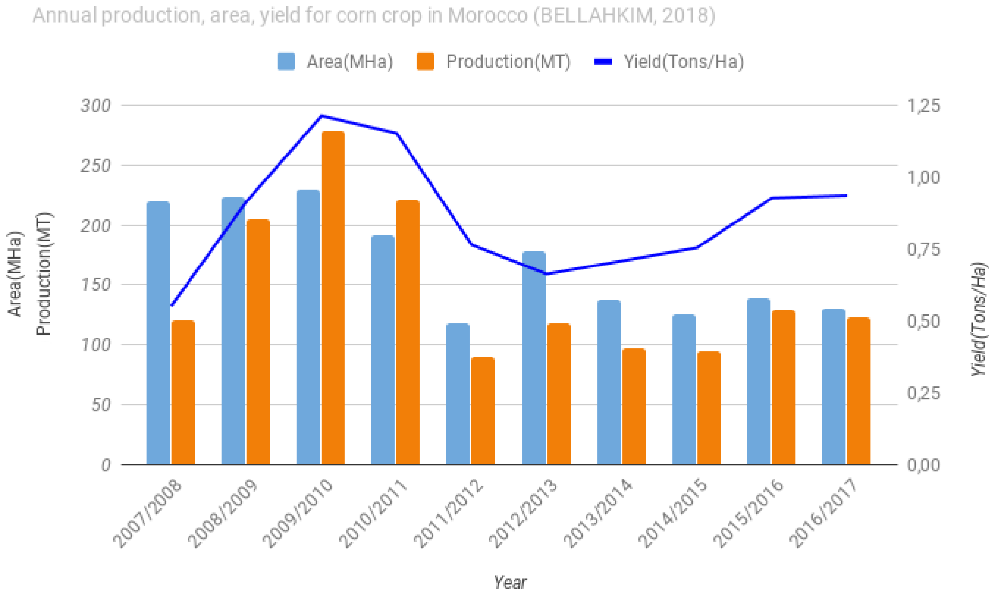

Figure 9: Annual production, area, the yield for the corn crop in Morocco (BELLAHKIM, 2020)

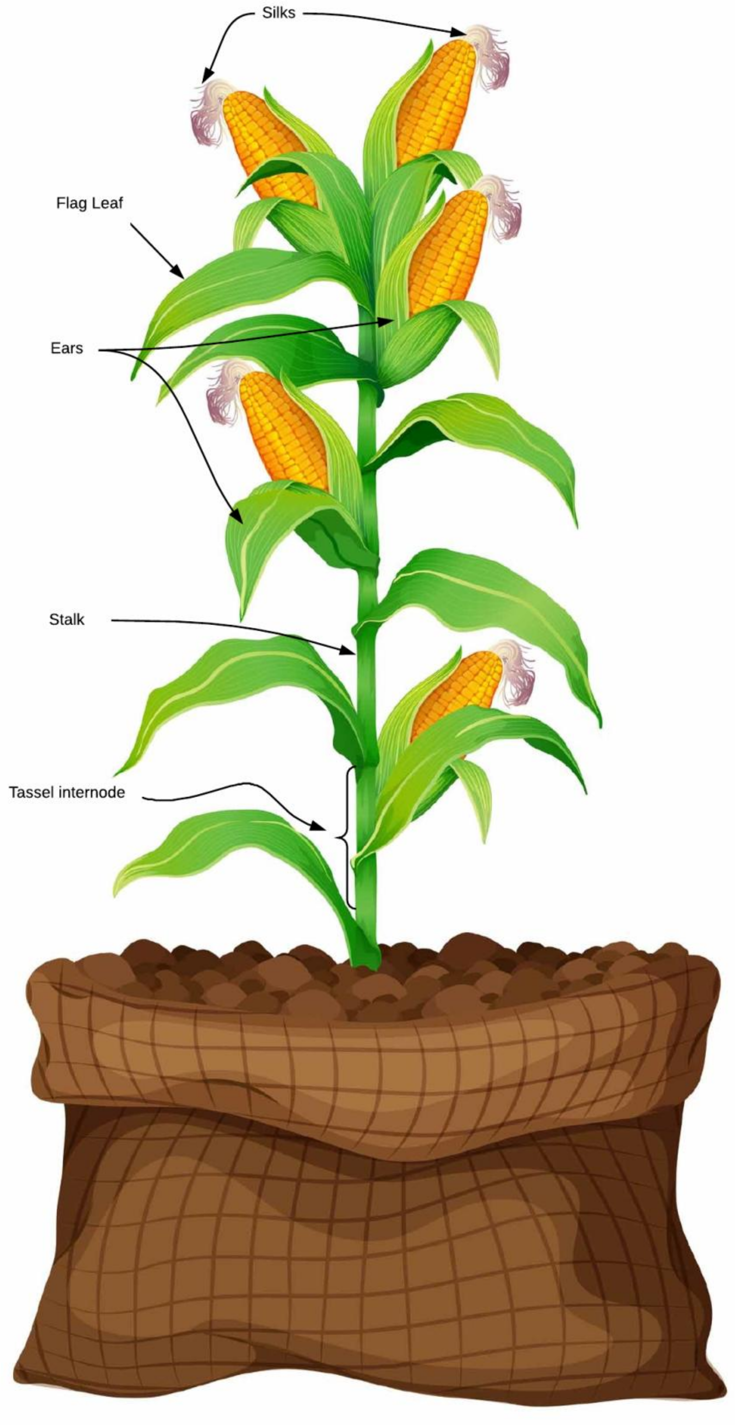

Figure 10: Corn plant (Photo from Freepik, designed by BELLAHKIM, 2020)

After the sharp drop in the production of maize crops in many regions in Morocco which was affected by the decrease of precipitation. the agricultural sector, due to its predominant place in the use of water resources. But lately, and since the 2013 year, there's been a slight increase in the production of this plant especially in the region of Grand Casablanca-Settat.

Mainly the main producer regions in Morocco are almost the Grand Casablanca-Settat region, followed by the region of Marrakech-Safi then the region of Rabat-Sale-Kenitra. According to data released by the minister of agriculture, the production of maize in Morocco in 2016/2017 in the region of Casablanca 54898 tons es was harvested from 56705 hectares.

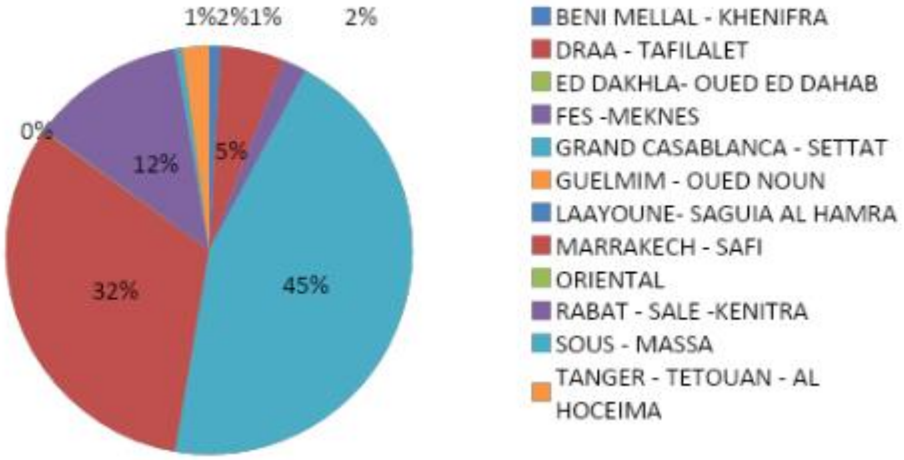

Figure 11: The production of maize in the year 2016/2017 (BELLAHKIM, 2020)

4.2.2. Corn residues

After the harvest of corn, the main residues are corn canes (or corn stalks), also called “corn straw”. Those are residues of the culture of corn. Made up of leaves and stems, as well as most often spathes and stalks, abandoned in the fields after the grain harvest. These residues represent approximately half by mass of the grain yield.

Data of residues is not easy to obtain, as opposed to what happens in crops. In this case, the most frequently used criterion is to estimate the ratio between the final product of the culture with their residues, it’s noted that recognizing that various factors will influence the ratio.

For maize residues, the whole crop residue is typically called corn stover, and its ratio varies from 0.9 to 1.1. Some data of these ratios are given in the *Table 6* below.

Table 6: Ratio between residue and grain for the corn crop

Residue	Ratio	Reference
Stover	1.0	(Ramachandra et al., 2004)
Stover	1.1	(Matsumura, 2005)
Stover	0.9-1.1	(Kadam & McMillan et al., 2003)

Cobs	0.15	(Zhang et al., 2012)
Leaves	0.22	(Zhang et al., 2012)
Stalks	0.50	(Zhang et al., 2012)

4.2.3. Use of corn residues

Corn residues can be used for several industrial applications such as the production of heat, litter, cellulose ethanol, furfural, etc. uses in the form of fuel, litter and fodder are applicable at the scale of an agricultural business.

4.2.3.1. Animal feed

Maize residues can be used for animals as a feed, especially in situations of a shortage of fodder. This plant has higher nutritional value than other crops such as wheat straw, they are used either in green in the form of pasture, or after chopping as silage intended to be used later, or to be harvested for a direct distribution (without silage). In the case of silage, the whole plant is used for that purpose (foliage and ears) which is chopped and then crushed between rollers during harvest. However, it is necessary to use dry matter with low content of mass solid (between 50-60%) to allow the process of conservation.

Table 7: Data reported in the literature for the composition of corn cob (%, dry basis)

Component	(Barl et al., 1991)	(Garrote et al., 2001)	(Tada et al., 2004)	(Nabarlatz et al., 2004)	(Moura et al., 2007)	(Kaliyan & Morey, 2010)	(Boonso-mbuti et al., 2013)
Cellulose	39.1	31.7	32.0	38.5	38.4	40.0	42.6
Hemicellulose	42.1	34.7	35.0	32.8	38.7	41.4	39.04
Lignin	9.1	20.3	20	18.7	12.3	5.8	7.56
Acetyl groupe	-	3.78	-	4.00	5.55	-	-
Ash	1.2	-	4	1.14	0.43	1.8	-
Extractives	-	-	-	2.1	-	-	-
Protein	1.7	-	-	-	3.40	2.5	-
Others	6.8	9.58	-	6.2	1.30	-	-

4.2.3.2. Animal litter

Residues generally have reduced protein content and digestible energy. The high levels of fibers insoluble in acid detergent (ADF) and of fibers insoluble in a neutral detergent (NDF) reveal that the fiber has a very low rate of digestibility, energy, and assimilation. The ash content of corn residue is presented in the bioenergy section. This parameter is important for animal feed, because, for each quantity of fiber ingested, the ash contains only minerals, but will not provide energy or protein. Instead of the use as livestock feed, maize straw can also be harvested for the use as bedding for or other livestock (i.e. used as cellulose mass to fix and contain the droppings animals) or can be used as plant manure which stays in the field and enriches the litter (used as green manure).

4.2.3.3. Agricultural amendment

When used as litter, they can be composted or removed and spread directly in the fields (in piles handled by mechanical loaders) for subsequent spreading in the fields. In the two cases, they end up as organic matter (OM) to improve soil fertility.

4.2.3.4. Bioenergy

Another use of corn cane is fuel for bioenergy or raw material for bioproducts. They can be burned in ovens for the production of electricity by steam turbines. They also can be used for the production of cellulosic ethanol, which is a biofuel produced from grasses, biomass, algae, or other plants.

The energy industry and farm machinery are planning a major use of biomass for ethanol production. The fibrous friction producing the most glucose during enzymatic hydrolysis would be the cob, followed by the leaves, and the stems. Enzymatic hydrolysis, using enzymes, breaks down lignocellulosic compounds (or NDF) into simple sugars like glucose. Ethanol is created by the fermentation of sugars and is concentrated by distillation. Many recent kinds of research have shown some bio-based products from corn such as bioethanol, acids (lactic, itaconic, succinic, and other) are obtained from corn syrup and other sugar sources. (Geiser et al., 2016; Ramos et al., 2016a)

Besides the social and economic pillar, the environment is one of the main pillars of sustainable development. It is based on the protection of ecosystems, by using renewable natural resources, to meet social needs, which are mainly provided by petroleum resources.

Bioproducts, or bio-based products, are products resulting from the development of biomass (renewable natural resources). They have functionality similar to that of fossil-based products, such as petroleum and natural gas, while providing environmental benefits. The *Table 8* summarizes some of the advantages and disadvantages of bio-sourced products.

Table 8: Some cons and pros of bio-based products.

Benefits	Disadvantages

Reducing greenhouse gas emissions: the case of biofuels.	Use of food resources (wheat, sugar cane, sunflower, etc).
Biodegradability: the case of biomaterials.	Depletion of water resources;
Recovery of organic waste (straw, the skin of vegetables and fruits, etc.	Upgrading technologies under development;
Reduction of dependence on petroleum resources.	Sometimes high prices.

In general, corn residues do not have a specific destination as an agricultural residue. But it can be used for a list of bioproducts which can be subdivided into three main categories such as bioenergy (we have talked before), the second way is biomaterials used in particular in the production of concrete for buildings, automobile door panels, and spare parts. And the third way of using this natural waste is biochemical products which can be used in painting, pharmaceutical, and bio-cosmetic.

Table 9: Bioproduct obtained from corn cobs

Valorization	Reference
Ethanol	(Beall et al., 1992; Chen et al., 2007; Itelima et al., 2013; Latif & Rajokz, 2001; Ramos et al., 2017)
Cellulose-based nanoparticles (as drug carrier)	(Kumar et al., 2010)
Xylitol	(Dominguez et al., 1997; El-Batal & Khalaf, 2004; Tada et al.,2004; Wang et al., 2011)
Itaconic acid	(Geiser et al., 2016; Ramos et al., 2016; Ramos et al., 2017)
Lactic acid	(Rivas et al., 2004)
Succinic acid	(Geiser et al., 2016; Ramos et al., 2016; Ramos et al., 2017)
Ferulic acid	(Torre et al., 2008)
Xylo-oligosaccharide	(Carvalheiro et al., 2009a; Garrote et al., 2002)
Activated carbon	(El-Sayed et al., 2014; Sun & Webley, 2010)
Glucaric acid (Saccharic)	(Vaishali et al., 2020)

Citric acid	(Hang & Woodams, 2001)

The *Table 9* shows some studies that have revealed the potential ways of using maize residues or the derived products that are already in the market (mainly in the USA).
A quote from the website corn.org that shows the importance of this natural renewable building block as the website has titled.
Corn is a versatile resource that can be used for just about everything – from making our food taste better and our cosmetics last longer, to making our plastics more environmentally friendly and our medicines easier to swallow.

Table 10: Summary of corn residue applications

Type of valorization	Specific application	Reference
Abrasive and Absorbent/ Cleaning	Refinishing and cleaning of natural wood homes…Cleaning carbon, oil as well as many products of corrosion from generic motor parts, cylinders, pistons...	(AGRISENT, 2014a; BestCobLLC, 2014)
Burnishing/ Polishing/ Deburr/ Deflash	Cleaning and polishing of ball bearing, nuts, and bolts… Computer chips, wire brads, jewelry, optical glass...	(AGRISENT, 2014a)
Agriculture/ Carrier	Mushroom cultivation, pharmaceutical carrier, pesticide carrier...	(BestCobLLC, 2014)
Absorbent	Antifreeze, absorbing rinse water in electroplated materials, sludge solidification, soil composting, animal bedding...	(AGRISENT ,2014b, 2014c; Morris, 2012, BestCobLLC, 2014)
Extender/ Filter	Filler for composite products, Plastic extender	(BestCobLLC, 2014)
Building material	Lightweight concrete for non-sturtural applications, Lightweight concrete masonry, Thermal insulation material	(Pinto et al., 2012; Faustino et al., 2015; Pinto et al., 2016)

- **Conclusion**

After the overview taken from the work of agricultural crops of maize production as well the product that we may extract from this natural resource, now we move to next chapter in which we will see one of the most important part which is the development of the anaerobic digestion model that will be the foundation of this work.

CHAPTER 2

DEVELOPMENT OF ANAEROBIC DIGESTION MODEL

• 1. Introduction

The modeling of the processes of anaerobic digestion, appeared at the end of the 1990s, constitutes an important line of research since it makes it possible to integrate in the same tool all the knowledge acquired on the bio-physico-chemical functioning of digestion media. The modeling aspect is a powerful tool for dynamic simulation of digestion media that can be use in a wide range of applications:

- Understanding of complex phenomena;
- Determination of certain kinetic parameters difficult to access by experimentation;
- Prediction of degradation kinetics, yields, dynamic evolution of environments;
- Quick comparison of different parameters.

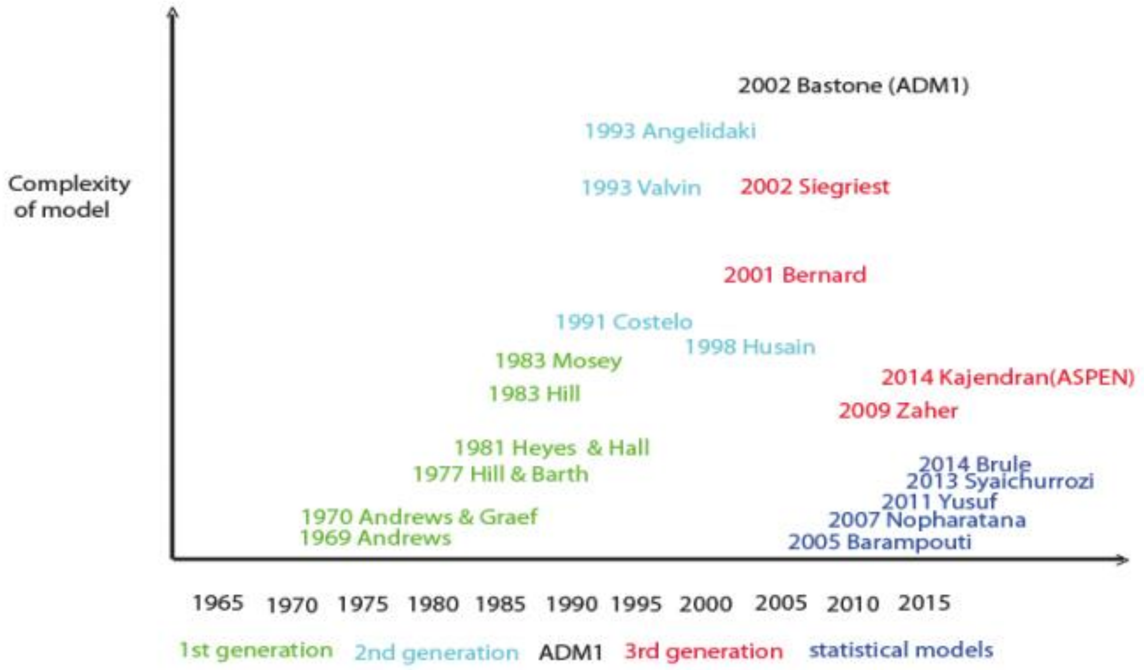

Figure 12: Evolution of AD models. Complexity over the last 50 years.

Table 11: Evolution of anaerobic digestion models – Generations

	1st generation (1969-1990)
Andrews, 1969	The first AD model was an inspired concept for other models.

	The bacterial growth inhibition was included using Haldane expression. The un-ionized acid was considered as the growth-limiting substrate.
Andrews and Graef, 1970	Was developed for the dynamic simulation of the enzymatic hydrolysis. Haldane kinetics was used for the description of the substrate digestion.
Hill and Barth, 1977	This model was created for poultry and swine waste using experimental data. Describing the AD process in only three phases: solubilization of organics,acidogenesis and methanogenesis.
Heyes and Hall, 1981	The AD model was performed, in which the process is affected by pH inhibition of methanogenesis and hydrogen inhibition of acetogens.
Hill, 1983	The AD model for the simulation of biogas and methane for poultry, beef and dairy waste. Hydrolysis is not included. Four state variables: volatile fatty acids (VFA); biodegradable volatile solids (BVS); acidogens and methanogens concentration.
Mosey, 1983	This model indicates four bacterial groups are responsible for AD of glucose to produce CH_4 and CO2. considering that hydrogen-partial pressure is the regulatory of metabolism.
	2nd generation (1991-2001)
Costello et al., 1991	This model was used to study the accumulation of lactic acid from glucose.
Angelidaki et al., 1993	This model was used to investigate the effects of ammonia in digestion media (manure).
Vavilin et al., 1994	Hydrolysis is considered as the rate-

	determining step for the digestion of swine waste, sewage sludge, cattle manure and cellulose.
Husain, 1998	The death rates of acidogens and methanogens are volatile fatty acid based on Monod functions.
	3rd generation (2001 - 2017)
Bernard et al., 2001	This model uses only two biodegradation steps (acidogenesis and methanogenesis). This model has 6 states and 30 parameters describing the AD process.
Siegrist et al., 2002	Simple model contains only a few inputs. The hydrolysis rate is defined by first-order kinetics. Excluding valerate and butyrate of the variable state.
	ADM1 (2002)
Batstone et al., 2002	The AD process is described in four steps: hydrolysis,acidogenesis, acetogenesis and methanogenesis which are related to the biochemical reactions.
Zaher et al., 2009	This model is for dairy waste, the whole process of AD is defined in four phases:hydrolysis, acidogenesis, methanogenesis (hydrogenotrophic and acetotrophic). The state variables used for the model are 15.
AD on ASPEN; A: Rajendran et al., 2014	This model uses 46 chemical reactions and inhibition phenomena, depending on the pH value.
Arzate et al., 2015	This model is based on the digestion of the energy crops such as maize, grass and clover silage.
	Statistical models
Barampouti et al., 2005	This model is dedicated for biogas

	production from potato processing wastewater.
Nopharatana et al., 2007	This model was used for AD of MSW. The hydrolysis process is expressed by the Contois function, while the Monod function used for acidogenesis, acetoclastic and methanogenesis.
Yusuf and Ify, 2011	The co-digestion of paper waste and cow dung with water hyacinth in five batch mode.
Syaichurrozi and Sumardiono, 2013	This model is based on the modified Gompertz equation to predict biogas production potential (BPP).
Brulé et al., 2014	This exponential model uses methane production In this model the hydrolysis phase is pretend to be much slower than the methane production step.

There are several models describing the processes of anaerobic digestion (<METHANE>, AM2, ADM1...etc). Since its establishment in 2002, the ADM1 model is the most widely used model in the field of anaerobic digestion because it is a complete kinetic model, integrating the main phenomena involved in the digestion media. Also, many changes have been made to the base model to refine the modeling of certain phenomena (inhibitions, disintegration/ hydrolysis, bacterial growth…). However, this model has been put in place for the modeling of biochemical processes of wet degradation. The physical, biological and kinetic parameters used therefore related to wet digestion processes and are poorly suited to dry processes. It is therefore necessary to adapt this global model to dry digestion, this technology being used more and more in industrial environments. The modeling work of the anaerobic digestion processes that we carried out is based on the model ADM1. The modifications made to this model as well as the implementation methods will be detailed later in the manuscript. The work done has several levels:

- Establishment of a global structure of the model (based on that of the ADM1)
- Determination of biological kinetic parameters that influence the digestion for the degradation steps selected (batch operation).

2. Model description

The model put in place is based on the ADM1 model. The ADM1 model is a structured biological model that describes the major mechanisms for converting a complex organic substrate into biogas and degradation by-products (Batstone et al., 2002; Parker, 2005, Yasui et al., 2008). In the ADM1 model, conversion of the complex organic matter is carried out according to the following scheme: the composite materials (complex substrates) are first converted into carbohydrates, proteins and lipids during the disintegration phase. These compounds are then hydrolysed into simple sugars, amino acids and long chain fatty acids. The next phase of acidogenesis converts these products from hydrolysis into fatty acids, acetic acid, hydrogen and carbon dioxide by the action of fermentative microorganisms. The fatty acids formed are then converted to acetate during the acitogenesis phase. Finally, the methanogenesis phase transforms acetate (acetoclastic methanogenesis) as well as hydrogen and carbon dioxide (hydrogenotrophic methanogenesis) into methane and carbon dioxide. The pattern of metabolic fluxes used in ADM1 is summarized in *Figure 14*.

The biological degradation is described by Monod-type equations in which the use of the substrates is coupled to the microbial growth. The phenomena of growth as well as many inhibition phenomena are taken into account in this model, a total of 24 state variables and 19 reactions (4 hydrolysis reactions, 8 substrate utilization reactions and 7 microbial population evolution reactions) are included in this model.

2.1. Principal modification to the ADM1 model

The biological conversion process of the complex organic molecules was through the breakdown into carbohydrates, proteins, and lipids (X_{ch}, X_{pro} and X_{li}) as a primary step of anaerobic digestion (Nordlander et al 2017).

For the purpose of simplicity, we have suggested a model originated from the ADM1 model, schematically, it's shown in *Figure 1*, whereas the original model has about 24 variables. Only that suggested model for this study, showing in *Figure 2* has only 6 variables (soluble component).

The state variables used are, therefore: soluble sugar(S_{su}), total butyrate (S_{bu}),total propionate (S_{pro}), total acetate (S_{ac}), soluble hydrogen (S_{H2}) and the finally soluble methane (S_{ch4}).

In this model, we consider that each of the following compounds (sugar, butyrate, propionate, acetate, hydrogen) has only one process of degradation which is the uptake process. As there's a proportional association between the growth of biomass and the uptake of the substrate. The mathematical model of the uptake process of substrate used is in the form of Monod functions to describe the kinetics of uptake of each compound, associated with pH, H_2 and NH_3 inhibition terms.

The complexity of the model ADM1 lies in the COD flow, also in the interconnection of the regeneration cycle and the decay of microorganisms. The production of (X_{ch}, X_{pro} and X_{li}) due to the decay of the majority of microorganisms which can be utilized as substrates after the first two phases of disintegration and enzymatic hydrolysis because of this regeneration, the model analysis becomes more complicated. Notwithstanding that the decay process could be ignored for simplification purposes.

In the model proposed we have used the glucose (sugar) as the key substrate, with only three phases of substrate degradation (acidogenesis, acetogenesis, and methanogenesis) instead of five phases by removing disintegration and hydrolysis.

We also decided to consider the microbial population as constant within the digestive media. This choice is motivated by the fact that in anaerobic digestion, the applied loads are low the microbial growth is minimal since less than 10 % of the substrate is transformed into biomass (Batstone et al., 2002). In addition, in industrial reactors, part of the biomass present in the outgoing digestate is recycled to the reactor head with the incoming waste. In continuous operation, the average amount of biomass present in the reactor is therefore substantially constant. This assumption is especially useful for the following reasons: it reduces the amount of state variables and kinetic parameters to be introduced into the model. Indeed, it is very difficult, if not impossible, to have access to precise population densities of the different trophic groups in the digestion media (i.e. acetogens, methanogens and hydrogenotrophic concentration). Consequently, for each i substrate used, the maximum rate of growth (k_m) and biomass concentration (X_i) were merged into a single (k_mX_i) parameter. This parameter, called "maximum substrate consumption rate", represents the activity of microorganisms degrading substrate "i". The hypothesis of a constant bacterial population is a strong assumption but has been put in place to allow the identification of parameters. A final major change to the model is the substrates that come into the model. As we can see from *Figure 13*, the ADM1 model takes into account 14 substrates and products: particulate matter, carbohydrates, proteins, lipids, amino acids, monosaccharides, long chain fatty acids (LCGA), acetate, propionate, butyrate, valerate, hydrogen, methane and carbon dioxide (plus inert soluble material which are however not state variables). We have greatly reduced the number of these substrates. Our model then integrates the following compounds: sugar, butyrate, acetate, propionate, hydrogen, methane. This reduction of the substrates has been possible thanks to the grouping of the disintegration, hydrolysis and acidogenesis stages which make it possible to overcome carbohydrates, proteins, lipids, amino acids, monosaccharides and AGLC (these compounds will be taken into account indirectly in the stoichiometry of degradation). In addition, the acidogenesis step theoretically forms various volatile fatty acids: acetate, propionate but also valerate and butyrate (Batstone, et al., 2002; Barnes and Keller, 2003; Paker, 2005; Yasui et al., 2008). In our model, valerate is not included because more than 90% of total VFAs consist of mesophilic acetate ,propionate and butyrate is often undetected or at very low levels (Skiadas et al., 2000; Hu et al., 2005). The metabolic fluxes taken into account in our model are detailed in *Figure 14*.

In summary, two main modifications have been make to the ADM1 model to best meet the specificities of dry anaerobic digestion:

- Microbial population considered constant and described by the parameter "k_mX_i";
- Reduction of the number of substrates and products, from 24 to 6.

2.2. Model unity

As for ADM1, the unit used in our model for the material balance is the COD (Chemical Oxygen Demand), a unit well adapted to the study of anaerobic processes. Molarity is used for compounds that do not have a COD such as dissolved CO_2 or bicarbonate HCO_3^-. However, the ADM1 which uses a unit volume (m^3), which is well adapted to the wet process. The units of the parameters used in the model are summarized in *Table 12*.

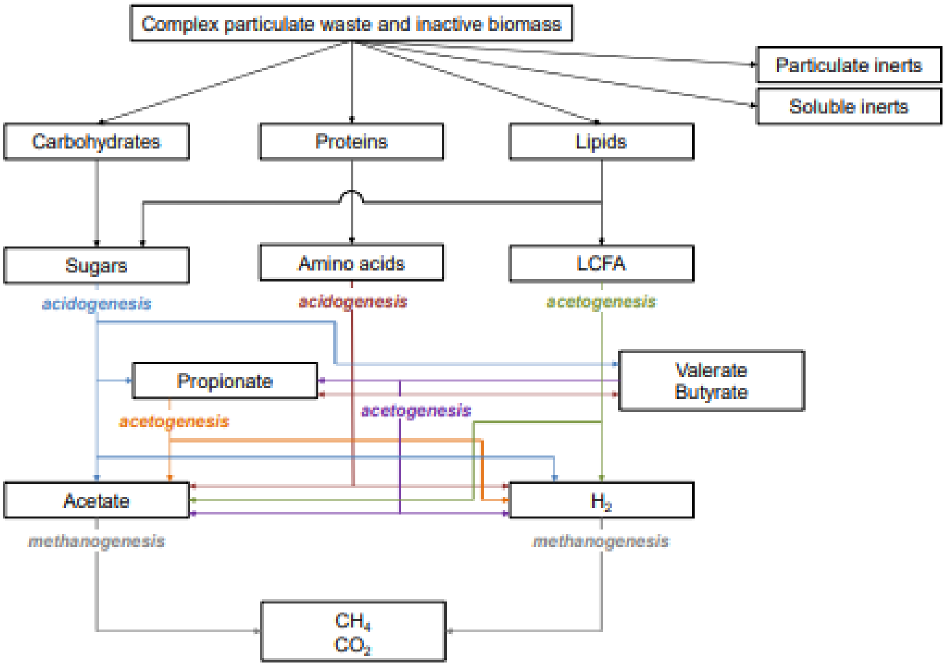

Figure 13: The anaerobic digestion process as described in Batstone et al. (2002)

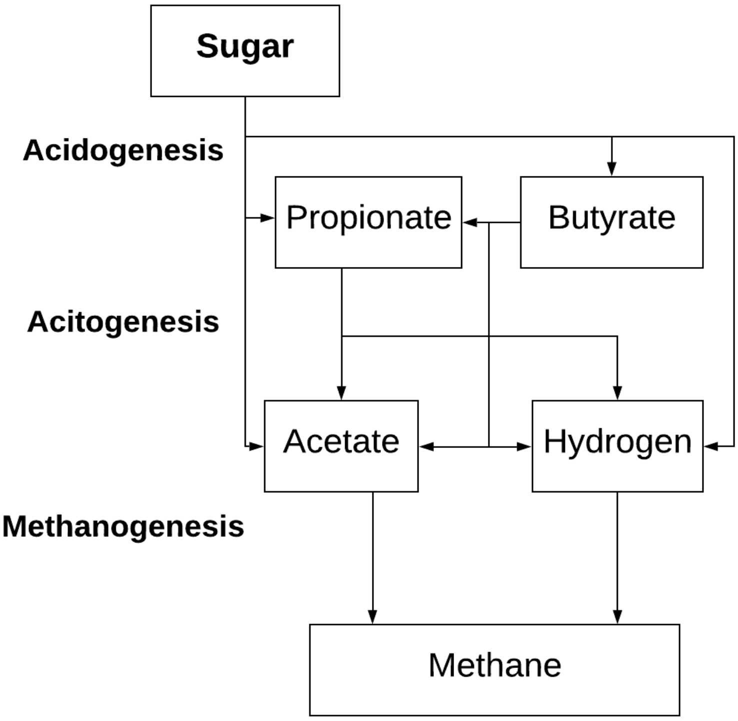

Figure 14: The modified ADM1 model used for the study

2.3. State variables

Table 12: Nomenclature and units used in the model

Symbol	Description	Units
i	Component index	
j	Process index	
S_i	Soluble component i	Nominally $kgCOD.m^{-3}$
$K_{s,i}$	Monod half saturation constant	$kgCOD.m^{-3}$
X_i	Particulate component i	$kgCOD.m^{-3}$
$k_{m,i}$	Specific Monod maximum uptake rate	$kgCOD.m^{-3}\_$ $S.kgCOD.m^{-3}\_X.d^{-1}$
$Y_{susbstrate}$	Yield of biomass on substrate	$kgCOD-X.kgCOD-S$
$f_{Product\ ,susbstrate}$	Yield (catabolism only) of product on substrate	$kgCOD.kgCOD^{-1}$
t	Time	d
I	Inhibition function	
K_I	Inhibition constant	Nominally $kgCOD.m^{-3}$
$K_{a/b}$	Acid-base rate constant for component i	$M^{-1}.d^{-1}$
K_a	Acid-base equilibrium constant	$M\ or\ (kmole.m^{-3})$

$k_L a$	Gas-liquid Monod maximum uptake rate	d^{-1}
K_H	Henry's law coefficient	$M.bar^{-1}$
V	Volume	m^3
q	Flow	$m^3.d^{-1}$
T	Temperature	k
$\nu_{i,j}$	Rate coefficient for componenti on process j	Nominally $kgCOD.m^{-3}$
ρ_i	Rate for process	$kgCOD.m^{-3}$

2.4. State variables

The sixth variables used in the model proposed are($S_{su}, S_{pro}, S_{bu}, S_{ac}, S_{H2}, S_{ch4}$). For the purpose of simplicity, we reduced the number of variables states from 24 variables (in the original paper of ADM1 proposed by the IWA in 2002) into 6, by neglecting the decay process.

2.5. Kinetics

The main constants and parameters of the model are summarized in *Table 13*. The mathematical model used in the modeling of the biological model of this investigation was through the differential equations in BATCH mode.

$$\frac{dS_{liq,j}}{dt} = \frac{Q}{V_{liq}} \cdot \left(S_{in,i} - S_{liq,i}\right) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \ ; i = 1,..,12;\ i = 25-26;$$

Also:

$$\frac{dX_{liq,j}}{dt} = \frac{Q}{V_{liq}} \cdot \left(X_{in,i} - X_{liq,i}\right) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \quad ;\ i = 13,...,24$$

2.6. Biogas production

The degradation products are obtained in their soluble form. The gaseous products are then obtained by transfer from the liquid phase to the gaseous phase. The production of biogas (CH_4, CO_2 and H_2) is then directly calculated from the concentrations in the liquid phase by dynamic equations of liquid-gas transfer as follows:

$$\frac{dS_{gas,i}}{dt} = -\frac{q_{gas}}{V_{gas}} S_{gas,i} + \frac{V_{liq}}{V_{gas}} \rho_{T,i} \ ;\ i = CH_4, CO_2, H_2$$

Where q_{gas} is the gas flow which denotes for the gas escapes from the head of the reactor; V_{liq} is the liquid reactor volume; V_{gas} is the gas reactor volume, $S_{gas,i}$ is the gas phase concentration of gas component i, $\rho_{T,i}$ is the specific mass transfer rate of gas "i" expressed as follows:

$$\rho_{T,i} = k_{La} \cdot \left(K_{H,i} \cdot P_{gas,i} - S_{liq,i} \right) \qquad ; i = CH_4, CO_2, H_2$$

Where $\rho_{liq\text{-}gas,i}$ is the specific transfer rate (mgCOD.kg^{-1}.d^{-1} or mmol.kg^{-1}.d^{-1} for IC), k_{La} is the overall transfer coefficient (d^{-1}), if is the concentration of compound i in the liquid (mgCOD.kg^{-1} or mmol.kg^{-1}.j^{-1} for IC), $K_{H,\,i}$ is Henry's constant of gas i (mmol.L^{-1}.bar^{-1}) and $P_{gas,i}$ is the partial pressure of the gas i (bar).

The transfer resistance of CH_4, CO_2 and H_2 is governed by the liquid film and their diffusivities are considered to be similar. Their liquid-gas transfer coefficients (k_{La}) are therefore of the same order of magnitude. The expression of the partial pressure of the gases, $P_{gas,i}$ is translated according to the equation below:

$$P_{gas,H_2} = S_{gas,H_2} \cdot \frac{R \cdot T_{op}}{16}$$

And:

$$P_{gas,CO_2} = S_{gas,CO_2} \cdot R \cdot T_{op}$$

Also :

$$P_{gas,CH_4} = S_{gas,CH_4} \cdot \frac{R \cdot T_{op}}{64}$$

The rate of gas production can be determined by using the equation. but in this case, the numerical solution of the problem may encounter many numerical problems. For that reason, an alternative equation is given in the report of Rosen to reduce numerical instability.

$$q_{gas} = k_p \left(P_{gas} - P_{atm} \right)$$

With

$$P_{gas} = P_{gas,H_2} + P_{gas,CH_4} + P_{gas,CO_2} + P_{gas,H_2O}$$

• 3. Integration

The implementation method in the case of a batch operation or a continuous operation is almost similar but has some modifications, especially in terms of material flow. Indeed, while the continuous model must necessarily simulate successive feeds and withdrawals, this is not the case in sequential operation since the only input term of the system is at the beginning of the simulation, in the form of a term. Representing the initial conditions. For the sake of clarity, we preferred to separate the implementation methods of the two types of operation.

Table 13: Petersen Matrix for soluble components

Components i ⟶ **Process j ↓**		**1** $\boldsymbol{S_{su}}$	**2** $\boldsymbol{S_{bu}}$	**3** $\boldsymbol{S_{pro}}$	**4** $\boldsymbol{S_{ac}}$	**5** $\boldsymbol{S_{H2}}$	**6** $\boldsymbol{S_{ch4}}$	**Rate** $\boldsymbol{\rho_j (kgCOD.m^{-3}.d^{-1})}$
1	Uptake of sugars	-1	$\eta_{bu,su}$	$\eta_{pro,su}$	$\eta_{ac,su}$	$\eta_{H2,su}$		$k_{m,su} X_{su} \frac{S_{su}}{K_{s,su}+S_{su}} I_5$
2	Uptake of butyrate		-1		$\eta_{ac,bu}$	$\eta_{H2,bu}$		$k_{m,bu} X_{c4} \frac{S_{bu}}{K_{s,c4}+S_{bu}} \frac{1}{1+\frac{S_{va}}{S_{bu}}} I_9$
3	Uptake of propionate			-1	$\eta_{ac,pro}$	$\eta_{H2,pro}$		$k_{m,pro} X_{pro} \frac{S_{pro}}{K_{s,pro}+S_{pro}} I_{10}$
4	Uptake of acetate				-1		$\eta_{ch4,ac}$	$k_{m,ac} X_{ac} \frac{S_{ac}}{K_{s,ac}+S_{ac}} I_{11}$
5	Uptake of hydrogen					-1	$\eta_{ch4,H2}$	$k_{m,h2} X_{h2} \frac{S_{H2}}{K_{s,H2}+S_{H2}} I_{12}$
		Monosaccharides (kgCOD.m^{-3})	**Total butyrate (kgCOD.m^{-3})**	**Total propionate (kgCOD.m-^{3})**	**Total acetate (kgCOD.m-^{3})**	**Hydrogen gas (kgCOD.m-^{3})**	**Methane gas (kgCOD.m-^{3})**	

Table 14: Values for stoichiometric and kinetic parameters used

Parameter		**Suggested value**	**Unity**
Stoichiometric	Y_{Su}	0.1	
	Y_{c4}	0.06	
	Y_{pro}	0.04	
	Y_{ac}	0.05	
	Y_{H2}	0.0282	
	$f_{bu,su}$	0.13	
	$f_{pro,su}$	0.27	
	$f_{ac,su}$	0.41	
	$f_{H2,su}$	0.19	

Kinetic	$K_{s,su}$	0.5-0.7	$kgCOD.m^{-3}$
	$K_{s,c4}$	0.2	$kgCOD.m^{-3}$
	$K_{s,pro}$	0.13	$kgCOD.m^{-3}$
	$K_{s,ac}$	0.09-0.15	$kgCOD.m^{-3}$
	$K_{s,H2}$	0.000007	$kgCOD.m^{-3}$
	$k_{m,su}$	20	d^{-1}
	$k_{m,c4}$	22	d^{-1}
	$k_{m,pro}$	13	d^{-1}
	$k_{m,ac}$	9.5	d^{-1}
	$k_{m,H2}$	8	d^{-1}

3.1. Implementation in sequential model (Batch)

If we consider that our reactor is on discontinuous mode in this case:

$$\frac{dS_{liq,j}}{dt} = \frac{Q}{V_{liq}} \cdot \left(S_{in,i} - S_{liq,i}\right) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \;\; ; i = 1,..,12;\; i = 25-26;$$

- We have **6 differential equations** for soluble components :

$$\frac{\partial S_{su}}{\partial t} = -\rho_{su} \tag{Eqt. 7}$$

$$\frac{\partial S_{bu}}{\partial t} = \eta_{bu,su}\rho_{su} - \rho_{bu} \tag{Eqt. 8}$$

$$\frac{\partial S_{pro}}{\partial t} = \eta_{pro,su}\rho_{su} - \rho_{pro} \tag{Eqt. 9}$$

$$\frac{\partial S_{H2}}{\partial t} = \eta_{H2,su}\rho_{su} + \eta_{H2,bu}\rho_{bu} + \eta_{H2,pro}\rho_{pro} - \rho_{H2} \tag{Eqt. 10}$$

$$\frac{\partial S_{ch4}}{\partial t} = \eta_{ch4,ac}\rho_{ac} + \eta_{ch4,H2}\rho_{H2} \tag{Eqt. 11}$$

Also the ADM1 gives us the possibility to integrate 3 dynamic equations of liquid-gas equilibria for CH_4, CO_2 and H_2 coupled to terms of outflow. The only term of creation corresponds to the amount of biogas resulting from the equilibrium liquid-gas equation, the output term corresponds to the withdrawal from the system. It comes:

$$\frac{dG_i}{dt} = \rho_{liq-gas,i}\frac{m_d}{V_{gas}} - G_i\frac{q_G}{V_{gas}} \qquad \text{Eqt. 12}$$

Where G_i is the gas phase concentration of compound i expressed in kg.COD.m^3

$$\frac{dG_i}{dt} = \frac{m_d}{V_{gas}}\left[\rho_{liq-gas,i} - G_i\frac{RT}{P_{atm}}\sum_{t}\rho'_{liq-gas,i}\right] \qquad \text{Eqt. 13}$$

It is possible to integrate in this expression a **gaseous retention factor** α_g representing the ratio of the gas volume to the total volume. This factor makes it possible to express the concentrations of gaseous species with respect to the gaseous volume. The gaseous retention factor is constant for a given reactor geometry. It comes then:

$$\frac{dG_i}{dt} = \frac{1-\alpha_g}{\alpha_g}d\left[\rho_{liq-gas,i} - G_i\frac{RT}{P_{atm}}\sum_{t}\rho'_{liq-gas,i}\right] \qquad \text{Eqt. 14}$$

Where d is the density of the digestate. This assessment, carried out on the 3 gaseous species makes it possible to write the three additional differential equations on the gaseous phase:

$$\frac{dG_{h2}}{dt} = -\frac{G_{h2}.q_{gas}}{V_{gas}} + \rho_{T,8}.\frac{V_{liq}}{V_{gas}} \qquad \text{Eqt. 15}$$

$$\frac{dG_{ch4}}{dt} = -\frac{G_{ch4}.q_{gas}}{V_{gas}} + \rho_{T,9}.\frac{V_{liq}}{V_{gas}} \qquad \text{Eqt. 16}$$

$$\frac{dG_{co2}}{dt} = -\frac{G_{co2}.q_{gas}}{V_{gas}} + \rho_{T,10}.\frac{V_{liq}}{V_{gas}} \qquad \text{Eqt. 17}$$

The biological component of the biogas production model describes the dynamics of the waste ecosystem. The principle of mass conservation of carbon is coupled with this model to link the different components of the model.

3.2. Implementation in continuous mode

The implementation in the continuous frame is strictly identical to that presented for the sequential operation with regard to gaseous compounds, that is to say for the state variables G_{CO2}, G_{CH4} and G_{H2}. In fact, the gaseous phase undergoes no modification during feed-withdrawal sequences. Equations of phase gas therefore remain unchanged during the transition to continuous operation.

On the other hand, all equations relating to the compounds present in the solid and liquid phase are modified.

Either a system operating in steady state and constant mass m_{dig}. Let Q_{in} and Q_{out} be the supply mass flow rates (in $m^3.d^{-1}$) and the withdrawal rates respectively ($Q_{in} = Q_{out} = Q$) since the mass of the system remains constant.

This modification is enough to model the behavior of a reactor which is supposed to be infinitely agitated.

4.3. Inhibition phenomena

Bacterial growth is not always possible, because it depends on the availability of nutrients, it is conditioned by the presence of predators, competing bacteria (competition) and in particular inhibitors.

The various bacterial populations included in ADM1 are revealed to be different types of inhibition, such as inhibition to pH or that is linked to the unavailability of nitrogen. Also, other inhibitors are related to the nature of some kinds of bacteria and their sensitivity to Hydrogen or Ammonia.

4.3.1. Inhibition by pH (Iph)

pH inhibition represents the combination of the destruction of homeostasis and an increase in the concentration of weak acids at low pH, or the growth of low base concentrations with transport limited to large pH, this affects in order:

Acetoclasts: Bacteria degrading acetate to produce methane, which is very sensitive to changes in pH.

Hydrogenotrophs: Those activities decrease when the acetate degrading cells are damaged.

The obligatory producers of hydrogen (X_{c4} and X_{pro}) their activities reduced due to the accumulation of H_2.

4.3.2. Inhibition by inorganic nitrogen (I_{IN})

Microorganisms use inorganic nitrogen to replenish their own nitrogen, they use it to replenish nitrogen from composites, soluble and particulate inert matter and proteins. Since the availability of nitrogen guarantees its recycling, limited quantities of this element limit the previous functions and cause the inhibition of bacterial colonies.

4.3.3. Inhibition by hydrogen (I_{H2})

Large concentrations of hydrogen can inhibit hydrogen-producing bacteria such as bacteria degrading valerate/butyrate and propionate, this is explained:

Since the enthalpy of acetate formation from propionate is positive, the biological reaction can only take place if the reaction products are consumed and knowing that a syntrophic relationship is required between acetogens and hydrogenophilus to avoid the blocking the metabolism of the latter; therefore high concentrations of hydrogen can cause the inhibition of acetogens and can even lead to bankruptcy of the digester if the excess hydrogen is not removed.

4.3.4. Inhibition by ammonia (I_{NH3})

This is a consequence of the increase in pH in a culture medium, which promotes the formation of ammonia NH_3 and hydrogen ions. Ammonia is toxic to microorganisms and causes deterioration of acetoclasts.

4.3.5. Inhibition equations

Different inhibition functions were suggested by the original ADM1 model to take into account the inhibition phenomena of substrates uptake processes either by decrease of pH below 7 or by shortage in inorganic nitrogen (I_{IN}) or by high concentrations of hydrogen (I_{h2}) or free ammonia nitrogen (I_{NH3}) during anaerobic fermentation. The implemented inhibition functions and the inhibition factors used in the ADM1 kinetic rate equations, updated by Rosen and Jeppsson (2005) are listed in *Table 15*.

Table 15: Inhibition functions and factors implemented in the original ADM 1

Description	Models
pH inhibition of step j	$I_{pH,i} = exp\left(-3\left(\frac{pH - pH_{UL,i}}{pH_{UL,i} - pH_{LL,i}}\right)^2\right)\ if\ pH < pH_{UL,i}$ $I_{pH,i} = 1\ if\ pH > pH_{UL,i}\ with\ i = aa, ac\ and\ h2.$
Inorganic nitrogen inhibition	$I_{IN,lim} = \frac{1}{1+\frac{K_{S,IN}}{S_{I,IN}}}$
Hydrogen inhibition	$I_{h2,i} = \frac{1}{1+\frac{S_{h2,i}}{K_{I,h2,i}}}\ with\ i = fa, c4\ and\ pro$
Free ammonia inhibition	$I_{NH3} = \frac{1}{1+\frac{S_{h2,IN}}{K_{I,NH3}}}$
Inhibition factors	$I_5 = I_{pH,aa} \cdot I_{IN,lim}$ $I_9 = I_{pH,aa} \cdot I_{IN,lim} \cdot I_{h2,c4}$ $I_{10} = I_{pH,aa} \cdot I_{IN,lim} \cdot I_{h2,pro}$ $I_{11} = I_{pH,aa} \cdot I_{IN,lim} \cdot I_{NH3}$ $I_{12} = I_{pH,aa} \cdot I_{IN,lim}$

4.4. Sensitivity of the different parameters

Since the modified ADM1 model deals with the anaerobic digestion of a single substrate (maize), its use for the co-digestion of two substrates or even the maize waste only will require the calibration of its parameters to better predict the behavior of the system. It is clear that adjusting all the parameters of the model is a difficult and time consuming task.

In this case, a sensitivity analysis is useful and necessary to determine the key parameters that strongly influence the model responses. It also makes it possible to identify and quantify the individual contributions of uncertain inputs to the output of the system (S.E. Jørgensen. 2016).

Among the 24 parameters of the modified ADM1 model, we only assess in what follows the influence of the fractionation coefficients and kinetic parameters, being directly related to bacterial growth and to biological conversion reactions (F. Mairet, et al, 2012).

The stoichiometric parameters defining the quantities of materials produced and degraded during the digestion process, as well as the physicochemical coefficients acting on the conversions of the chemical material are therefore not taken into account during the sensitivity study.

• Conclusion

ADM1-type models are nonetheless very complex models, the control of which remains impossible unless they are reduced to simpler models such as the modified ADM1 model.

In the next chapter, we propose the mathematical equations of different models used for the modeling of anaerobic digestion of maize waste as the physical model used for mass energy and energy conservation or mass transfert.

CHAPTER 3

MATHEMATICAL FORMULATIONS

• 1. Introduction

The mathematical model descripting the physical phenomena developed from the conservation equations of mass and energy written for each component (liquid, gas). By considering waste as a reactive porous medium. A model of biogas production depending both on the nature of the waste, on temperature and humidity. We present a model of two-phase flows without phase change. For this, we present the conservation equations of matter and energy and the thermodynamic functions. By adopting the following assumptions:

- The type of waste is Maize.
- The use of the laws of capillary pressure and permeability.
- The liquids are immiscible and incompressible.
- The medium is porous with constant porosity.
- The flow is laminar and described by generalized Darcy law.
- The gas is perfect.
- The fluids (gases, liquids) are Newtonian modeled by arrhenius' law.

• 2. Generalized Darcy's law

The velocities of the fluid phases flowing in a porous medium can be expressed using the generalized Darcy law:

$$v_i = -\frac{k_{i,p} k_{r,p}}{\mu_i} (\nabla P_i - \rho_i g)$$

Where, $K_{i,p}$, $K_{r,p}$ μ_p and P_i are respectively the intrinsic and relative permeabilities, the dynamic viscosity and the pressure of each phase (liquid, gas).
The density of the gas is defined as follows:

$$\rho_g = \frac{M_g P_g}{RT}$$

Where M_g is the molar mass of the gas (kg / mol), R (J / mol.K) the universal constant of ideal gases and T(K) is the temperature.

• 3. Mass conservation

Consider the case where the porous medium consists of the solid matrix, a liquid and a gas. The conservation of each of the constituents (liquid, gas) is written:

$$\begin{cases} \dfrac{\partial m_l}{\partial t} + \nabla.(\rho_l . v_l) = 0 \\ \dfrac{\partial m_g}{\partial t} + \nabla(\rho_g . v_g) = \alpha_g \end{cases} \qquad (I)$$

Also we know: $m_l = n \cdot S_l . \rho_l$ and $m_g = n.(1 - S_l). \rho_g$

Where n is the porosity of the medium, S_l is the liquid saturation and ρ_p the density of the liquid and gas phases. V_p the filtration rate of phase P defined by Darcy's law and α_g the term of biogas production. The latter term is defined from the biological model of degradation and production of biogas.

$$\begin{cases} n.\rho_l.\dfrac{\partial S_l}{\partial t} + \rho_l.\nabla.\left(-\dfrac{ki_{l.}k_{rl}}{\mu_l}(\nabla P_l - \rho_l\, \vec{g})\right) = 0 \\ n.\dfrac{\partial \rho_g}{\partial t}.(1 - S_l) + \nabla.\left(-\rho_g.\dfrac{k_{ig.}k_{rg}}{\mu_g}(\nabla P_g - \rho_g \vec{g})\right) = \alpha_g \end{cases} \quad \text{(II)}$$

The projection of the system of equations (II) following the cylindrical coordinate system while noting that:

$$\begin{cases} n.\dfrac{\partial S_l}{\partial t} = \dfrac{k_{il.}}{\mu_l}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}\left(r.k_{rl}.\rho_g.\dfrac{\partial P_l}{\partial r}\right) + \dfrac{\partial}{\partial z}\left(k_{rg}.\rho_g(\dfrac{\partial P_l}{\partial z} - \rho_l g)\right)\right)\right] \\ n.(1 - S_l).\dfrac{\partial \rho_g}{\partial t} - n.\rho_g.\dfrac{\partial S_l}{\partial t} - \dfrac{k_{ig.}}{\mu_g}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}\left(r.k_{rg}.\rho_g.(\dfrac{\partial P_g}{\partial r} - \rho_l g)\right) + \dfrac{\partial}{\partial z}\left(k_{rg}.\rho_g(\dfrac{\partial P_g}{\partial z} - \rho_g g)\right)\right)\right] = \alpha_g \end{cases}$$

We put

$$\begin{cases} W' = \dfrac{k_{il.}}{\mu_g}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}\left(r.k_{rl}.\rho_g.\dfrac{\partial P_l}{\partial r}\right) + \dfrac{\partial}{\partial z}\left(k_{rg}.\rho_g\left(\dfrac{\partial P_l}{\partial z} - \rho_l g\right)\right)\right)\right] \\ A = n.(1 - S_l).\dfrac{\partial \rho_g}{\partial t} - n.\rho_g.\dfrac{\partial S_l}{\partial t} \end{cases}$$

As well:

$$\begin{cases} n.\dfrac{\partial S_l}{\partial t} = W' & \textbf{(1)} \\ A - \dfrac{k_{ig.}}{\mu_g}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}\left(r.k_{rg}.\rho_g.\dfrac{\partial P_g}{\partial r} - r.k_{rg}.{\rho_g}^2.g)\right) + \dfrac{\partial}{\partial z}\left(k_{rg}.\rho_g.\dfrac{\partial P_g}{\partial z} - k_{rg}.{\rho_{g.}}^2 g\right)\right)\right] = \alpha_g & \textbf{(2)} \end{cases}$$

With:

$$\begin{cases} W' = \dfrac{k_{il.}}{\mu_g}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}(r.k_{rl}.\rho_g.f_{lr}) + \dfrac{\partial}{\partial z}(k_{rg}.\rho_g.f_{lz})\right)\right] \\ A - \dfrac{k_{ig.}}{\mu_g}\left[\left(\dfrac{1}{r}.\dfrac{\partial}{\partial r}\left(r.k_{rg}.\rho_g.\dfrac{\partial P_g}{\partial r} - r.k_{rg}.{\rho_g}^2.g)\right) + \dfrac{\partial}{\partial z}\left(k_{rg}.\rho_g.\dfrac{\partial P_g}{\partial z} - k_{rg}.{\rho_{g.}}^2 g\right)\right)\right] = \alpha_g \end{cases}$$

We make the following suggestions: $\begin{cases} f_{lr} = \dfrac{\partial P_l}{\partial r} \\ f_{gr} = \dfrac{\partial P_g}{\partial r} \end{cases}$ and $\begin{cases} f_{lz} = (\dfrac{\partial P_l}{\partial z} - \rho_l g) \\ f_{gz} = \dfrac{\partial P_g}{\partial z} \end{cases}$

$$\begin{pmatrix} \frac{1}{r}.k_{rg}.\rho_g.f_{gr} \\ +f_{gr}.k_{rg}.\frac{\partial \rho_g}{\partial r} \\ +f_{gr}.\rho_g.\frac{\partial k_{rg}}{\partial r} \\ +\rho_g.k_{rg}.\frac{\partial f_{gr}}{\partial r} \end{pmatrix} - \begin{pmatrix} \frac{1}{r}.k_{rg}.{\rho_g}^2.g \\ +{\rho_g}^2.g.\frac{\partial k_{rg}}{\partial r} \\ +g.k_{rg}.2\rho_g.\frac{\partial \rho_g}{\partial r} \\ . \end{pmatrix} + \begin{pmatrix} k_{rg}.f_{gz}.\frac{\partial \rho_g}{\partial z} \\ +f_{gz}.\rho_g.\frac{\partial k_{rg}}{\partial z} \\ +k_{rg}.\rho_g.\frac{\partial f_{gz}}{\partial z} \\ . \end{pmatrix} - \begin{pmatrix} g.k_{rg}.2\rho_g.\frac{\partial \rho_g}{\partial z} \\ +g.{\rho_g}^2.\frac{\partial k_{rg}}{\partial r} \end{pmatrix} = (A-\alpha_g).\frac{k_{ig}}{\mu_g}$$

- ## 4. Model of waste degradation and production of biogas

In the Maize waste used in our simulation, we have considered that our residues have contained a big amount of carbohydrates, with small quantities of lipids and fat. Therefore, we have used sugar (glucose) as the key substrate in our organic waste.

4.1 Application to the ADM1 model

If we consider that our reactor is on discontinuous mode in this case, we assume that q_{in} is different than q_{out}.

$$\frac{dS_{liq,j}}{dt} = \frac{Q}{V_{liq}} \cdot \left(S_{in,i} - S_{liq,i}\right) + \sum_{j=1-19} \rho_j \upsilon_{i,j} \;; i = 1,..,12;\; i = 25-26;$$

We have 6 differential equations for soluble components S_i:

$$\frac{\partial S_{su}}{\partial t} = -\rho_{su}$$
$$\frac{\partial S_{bu}}{\partial t} = \eta_{bu,su}\rho_{su} - \rho_{bu}$$
$$\frac{\partial S_{pro}}{\partial t} = \eta_{pro,su}\rho_{su} - \rho_{pro}$$
$$\frac{\partial S_{ac}}{\partial t} = \eta_{ac,su}\rho_{su} + \eta_{ac,bu}\rho_{bu} + \eta_{ac,pro}\rho_{pro} - \rho_{ac}$$
$$\frac{\partial S_{H2}}{\partial t} = \eta_{H2,su}\rho_{su} + \eta_{H2,bu}\rho_{bu} + \eta_{H2,pro}\rho_{pro} - \rho_{H2}$$
$$\frac{\partial S_{ch4}}{\partial t} = \eta_{ch4,ac}\rho_{ac} + \eta_{ch4,H2}\rho_{H2}$$

4.1.1 Water phase equations

- Production rate of sugar

$$\frac{\partial S_{su}}{\partial t} = -k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su} + S_{su}}$$

- Production rate of butyrate

$$\frac{\partial S_{bu}}{\partial t} = (1-Y_{Su}) \times f_{bu,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su}+S_{su}} - k_{m,c4} \times X_{c4} \times \frac{S_{bu}}{K_{s,c4}+S_{bu}} \times \frac{1}{1+\frac{S_{va}}{S_{bu}}}$$

- Production rate of propionate

$$\frac{\partial S_{pro}}{\partial t} = (1-Y_{Su}) \times f_{pro,su} \times X_{su} \times k_{m,su} \frac{S_{su}}{K_{s,su}+S_{su}} - k_{m,pro} \times X_{pro} \times \frac{S_{pro}}{K_{s,pro}+S_{pro}}$$

- Production rate of acetate

$$\begin{aligned}\frac{\partial S_{ac}}{\partial t} = {} & (1-Y_{Su}) \times f_{ac,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su}+S_{su}} + (1-Y_{c4}) \times 0{,}8 \times k_{m,c4} \times X_{c4} \\ & \times \frac{S_{bu}}{K_{s,c4}+S_{bu}} \times \frac{1}{1+\frac{S_{va}}{S_{bu}}} + (1-Y_{pro}) \times 0{,}57 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}}{K_{s,pro}+S_{pro}} \\ & - k_{m,ac} \times X_{ac} \times \frac{S_{ac}}{K_{s,ac}+S_{ac}}\end{aligned}$$

- Production rate of hydrogen

$$\begin{aligned}\frac{\partial S_{H2}}{\partial t} = {} & (1-Y_{Su}) \times f_{H2,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su}+S_{su}} + (1-Y_{c4}) \times 0{,}2 \times k_{m,c4} \times X_{c4} \\ & \times \frac{S_{bu}}{K_{s,c4}+S_{bu}} \times \frac{1}{1+\frac{S_{va}}{S_{bu}}} + (1-Y_{pro}) \times 0{,}43 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}}{K_{s,pro}+S_{pro}} \\ & - k_{m,H2} \times X_{H2} \times \frac{S_{H2}}{K_{s,H2}+S_{H2}}\end{aligned}$$

- Production rate of methane

$$\frac{\partial S_{ch4}}{\partial t} = (1-Y_{ac}) k_{m,ac} \times X_{ac} \times \frac{S_{ac}}{K_{s,ac}+S_{ac}} + (1-Y_{H2}) \times k_{m,H2} \times X_{H2} \times \frac{S_{H2}}{K_{s,H2}+S_{H2}}$$

4.1.2 Gas phase equations

$$\frac{dS_{gas,i}}{dt} = -\frac{q_{gas}}{V_{gas}} S_{gas,i} + \frac{V_{liq}}{V_{gas}} \rho_{T,i} \quad ; i = CH_4, CO_2, H_2$$

With:

$$\rho_{T,i} = k_{La} \cdot \left(K_{H,i} \cdot P_{gas,i} - S_{liq,i}\right) \qquad ; i = CH_4, CO_2, H_2$$

Eqt. 18

And

$$P_{gas} = P_{gas,H_2} + P_{gas,CH_4} + P_{gas,CO_2} + P_{gas,H_2O} \qquad \textit{Eqt. 19}$$

Also we have the pression expressions of different gases CH_4, H_2 and CO_2.

$$P_{gas,CH_4} = S_{gas,CH_4} \cdot \frac{R \cdot T_{op}}{64} \qquad \textit{Eqt. 20}$$

$$P_{gas,H_2} = S_{gas,H_2} \cdot \frac{R \cdot T_{op}}{16} \qquad \textit{Eqt. 21}$$

$$P_{gas,CO_2} = S_{gas,CO_2} \cdot R \cdot T_{op} \qquad \textit{Eqt. 22}$$

As we know:

$$q_{gas} = k_p \left(P_{gas} - P_{atm} \right) \qquad \textit{Eqt. 23}$$

With k_p is the friction of biogas in the gas outlet.

4.2 Energy conservation

We are interested in the theoretical modeling of the law of conservation of energy in a reactive porous medium (homogeneous, isotropic and indeformable), occupied by two fluid phases (water and gas), possibly consisting of several species Christophe Aran (C.Aran al, 2000) .

$$\sum_i^{l,g} h_i \left(\frac{\partial \rho_i}{\partial t} + \nabla.(\rho_i.v_i) \right) + \sum_i^{l,g} \rho_i.v_i.\nabla h_i + \sum_i^{l,g} \rho_i \frac{\partial h_i}{\partial t} = \nabla.(\lambda^*.\nabla \mathrm{T}).\alpha_q$$

We can writed as follow:

$$A = h_l \left(\frac{\partial \rho_l}{\partial t} + \rho_l \frac{k_{il.}}{\mu_l} \left[\left(\frac{1}{r}.\frac{\partial}{\partial r} \left(r.k_{rl}.\rho_g.\frac{\partial P_l}{\partial r} \right) + \frac{\partial}{\partial z} \left(k_{rg}.\rho_g \left(\frac{\partial P_l}{\partial z} - \rho_l g \right) \right) \right) \right] \right) +$$

$$h_g \left(\frac{\partial \rho_g}{\partial t} + \rho_g \frac{k_{ig.}}{\mu_g} \left[\left(\frac{1}{r}.\frac{\partial}{\partial r} \left(r.k_{rg}.\rho_g.\left(\frac{\partial P_g}{\partial r} - \rho_l g \right) \right) + \frac{\partial}{\partial z} \left(k_{rg}.\rho_g \left(\frac{\partial P_g}{\partial z} - \rho_g g \right) \right) \right) \right] \right)$$

$$B = \rho_l.v_l.\nabla h_l + \rho_g.v_g.\nabla h_g$$

$$\nabla h_l = \frac{\partial h_l(T)}{\partial t}.\nabla(\mathrm{T}) = \frac{\partial h_l(T)}{\partial T}\frac{\partial T}{\partial t} = C_{pl}(T).\nabla(\mathrm{T})$$

$$B = \left(\rho_l.\frac{k_{il}k_{rl}}{\mu_l}(\nabla P_l - \rho_l g)\right).C_{pl}(T).\nabla(\mathrm{T}) + \left(\rho_g.\frac{k_{ig}k_{rg}}{\mu_g}(\nabla P_g - \rho_g g)\right).C_{pg}(T).\nabla(\mathrm{T})$$

$$C = \rho_l.\frac{\partial h_l(T)}{\partial t} + \rho_g.\frac{\partial h_g(T)}{\partial t} = \rho_l.C_{pl}(T).\frac{\partial T}{\partial t} + \rho_g.C_{pg}(T).\frac{\partial T}{\partial t} = \left(\rho.C_p(T)\right)^*.\frac{\partial T}{\partial t}$$

$$D = \nabla.\left(\lambda^*.(\frac{\partial T}{\partial z} + \frac{\partial T}{\partial r})\right) = \lambda^*\left(\frac{\partial^2 T}{\partial z^2} + \frac{1}{r}.\frac{\partial T}{\partial r}\left(\frac{r\partial T}{\partial z}\right)\right)$$

Or we can use the follwing:

$$\left(\rho C_p\right)^*\frac{\partial T}{\partial t} + \overrightarrow{Up}\left(\rho C_p\right)_f \nabla T = \nabla(\lambda^*\nabla T) + Q$$

We can also writed Up as the following:

$$\overrightarrow{Up} = U_{p1}\overrightarrow{e_r} + U_{p2}\overrightarrow{e_z}$$

Which can become:

$$\left(\rho C_p\right)^*\frac{\partial T}{\partial t} + \left(\rho C_p\right)_f\left(U_{p1}\frac{\partial T}{\partial r} + U_{p2}\frac{\partial T}{\partial z}\right) = \frac{\lambda^*}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \lambda^*\frac{\partial^2 T}{\partial z^2} + Q \qquad \text{(III)}$$

With :

$$\lambda^* = (1-n)\lambda_s + n\lambda_f$$

And :

$$\left(\rho C_p\right)^* = \left(\rho C_p\right)_l.\theta_l + \left(\rho C_p\right)_g\theta_g$$

λ^*(W.m^{-1}.K^{-1}) is the equivalent thermal conductivity of the considered three-phase system.

• Conclusion

To be able to model the biological phenomena during the anaerobic degradation of waste, we must first know these phenomena, the different phases of degradation, the families of microorganisms that participate in each phase and the parameters, as well the important processes that influence waste degradation and biogas production, such as water content, temperature, leachate recirculation, as well the ADM1 parameter that also has a slight influence on the production biogas.

We present here the equations reflecting the conservation of mass, energy as well as the equations of biodegradation, generally these equations do not admit analytical solutions which require the use of numerical methods for the resolution of differential equations. For this we have opted to use the finite volume method for the conservation of mass and energy equations, and the Runge-Kutta method for the biodegradation equations.

CHAPTER 4

RESOLUTION METHOD

• 1. Introduction

In the present simulation, we have opted to use the finite volume method and the implicit Runge-Kutta method. The finite volume method is a discretization method well suited to the numerical resolution of conservation equations of extensive quantities. This method has various properties such as local conservation of flows, respect for the maximum principle, the possibility of applying it to any meshes (structured or unstructured meshes) which make it attractive. Another advantage of this method is that it leads to robust digital schemes. This explains why this method is widely used in various fields: fluid mechanics, heat and mass transfer, reservoir simulation in petroleum engineering, etc.
These methods require two steps: meshing and discretization.

• 2. Mesh

In two dimensions, the domain is subdivided into a finite number of control volumes which are made up of regular surface elements.
The mesh has the following form:

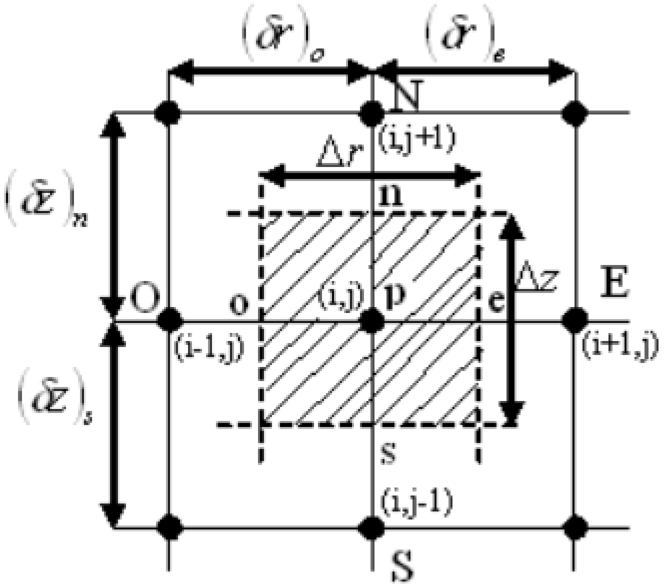

Figure 15: Mesh for finite-element method

Where: P is the main node, i the discretization index along the "r" axis, j the discretization index along the "z" axis.

The time will be indexed by the index "k". In general, the letters E, O, N and S represent East, West, North and South respectively.

The square colored in light blue represents a control volume element.
The segments [PE] and [PN] are respectively Δr and Δz.
Subsequently, we will adopt the following meshes:

$$r(i)=(i-1)\Delta r$$
$$z(i)=(j-1)\Delta z$$

• 3. Discretization

3.1 Mass conservation

By integrating equation (1) following the control volume (rdrdz) and along the time interval of length dt, it comes:

$$\iiint_t^{dt+t} nr\frac{\partial S_l}{\partial t}dtdrdz = \iiint_t^{dt+t}\frac{K_{il}}{\mu_l}\frac{\partial}{\partial \mathrm{r}}\left(rK_{r,l}f_{lr}\right)dtdrdz + \iiint_t^{dt+t}\frac{K_{il}}{\mu_l}\frac{\partial}{\partial \mathrm{z}}\left(K_{r,l}f_{lz}\right)r\,dtdrdz \qquad (3)$$

By calculating term by term, the integrals of the above equation lead to:

$$\iiint_t^{dt+t} nr\frac{\partial S_l}{\partial t}dtdrdz = nr_p\left(S_{l_p}^{dt+t} - S_{l_p}^{t}\right)\Delta r\Delta z$$

$$\iiint_t^{dt+t}\frac{K_{il}}{\mu_l}\frac{\partial}{\partial \mathrm{r}}\left(rK_{r,l}f_{lr}\right)rdtdrdz = \frac{K_{il}}{\mu_l}\left[\frac{\partial}{\partial \mathrm{r}}\left(rK_{r,l}f_{lr}\right)\right]_p^{dt+t}\Delta r\Delta z\Delta t$$

$$\iiint_t^{dt+t} r\frac{K_{il}}{\mu_l}\frac{\partial}{\partial \mathrm{z}}\left(K_{r,l}f_{lz}\right)dtdrdz = \frac{K_{il}}{\mu_l}r_p\left[\frac{\partial}{\partial \mathrm{z}}\left(K_{r,l}f_{lz}\right)\right]_p^{dt+t}\Delta r\Delta z\Delta t$$

By introducing the indices i and j it comes :

$$nr_p\left(S_{l_{(i,j)}}^{dt+t} - S_{l_{(i,j)}}^{t}\right)\Delta r\Delta z = \frac{K_{il}}{\mu_l}\left[\frac{\partial}{\partial \mathrm{r}}\left(rK_{r,l}f_{lr}\right)\right]_{(i,j)}^{dt+t}\Delta r\Delta z\Delta t + \frac{r_pK_{il}}{\mu_l}\left[\frac{\partial}{\partial \mathrm{z}}\left(K_{r,l}f_{lz}\right)\right]_{(i,j)}^{dt+t}\Delta r\Delta z\Delta t$$

Or :

$$\boldsymbol{S_{l_{(i,j)}}^{dt+t} = S_{l_{(i,j)}}^{t} + \frac{K_{il}}{r_p n\mu_l}\left[\frac{\partial}{\partial \mathrm{r}}\left(rK_{r,l}f_{lr}\right)\right]_{(i,j)}^{dt+t}\Delta t + \frac{K_{il}}{n\mu_l}\left[\frac{\partial}{\partial \mathrm{z}}\left(K_{r,l}f_{lz}\right)\right]_{(i,j)}^{dt+t}\Delta t} \qquad \textbf{(4)}$$

Also we did the same thing by integrating equation (2) following the control volume (rdrdz) and along the time interval of length dt, it comes:

$$\int_{k}^{k+1} n(1-S_l)\frac{\partial \rho_g}{\partial t} rdrdzdt - \int_{k}^{k+1} \rho_g W rdrdzdt - \int_{k}^{k+1} \frac{K_{ig}}{r\mu_g}\frac{\partial}{\partial \mathrm{r}}\left(r\rho_g K_{r,g} f_g\right) rdrdzdt + \int_{k}^{k+1} \frac{gK_{ig}}{r\mu_g}\frac{\partial}{\partial \mathrm{r}}(r{\rho_g}^2 K_{r,g}) rdrdzdt - \int_{k}^{k+1} \frac{K_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{z}}\left(\rho_g K_{r,g} f_g\right) rdrdzdt + \int_{k}^{k+1} \frac{gK_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{z}}({\rho_g}^2 K_{r,g}) rdrdzdt = \int_{k}^{k+1} \alpha_g rdrdzdt$$

$$\int_{k}^{k+1} n(1-S_l)\frac{\partial \rho_g}{\partial t} rdrdzdt = n\left(1-{S_l}_p^k\right)\left({\rho_g}_p^{k+1} - {\rho_g}_p^{k}\right) r_p \Delta r \Delta z$$

$$\int_{k}^{k+1} \rho_g W rdrdzdt = {\rho_g}_p^{k} W_p^{k+1} r_p \Delta r \Delta z \Delta t$$

$$\int_{k}^{k+1} \alpha_g rdrdzdt = {\alpha_g}_p^{k+1} r_p \Delta r \Delta z \Delta t$$

Also :

$$\int_{k}^{k+1} \frac{K_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{r}}\left(r\rho_g K_{r,g} f_g\right) drdzdt = \frac{K_{ig}}{\mu_g}\left(\left(r\rho_g K_{r,g} f_g\right)_e^{k+1} - \left(r\rho_g K_{r,g} f_g\right)_o^{k+1}\right)\Delta z \Delta t = \frac{K_{ig}}{2\mu_g}\left(\left(\rho_g\right)_E^{k+1}\left(rK_{r,g} f_g\right)_E^{k+1} - \left(\rho_g\right)_O^{k+1}\left(rK_{r,g} f_g\right)_O^{k+1}\right)\Delta z \Delta t$$

$$\left(r\rho_g K_{r,g} f_g\right)_e^{k+1} = \frac{\left(r\rho_g K_{r,g} f_g\right)_E^{k+1} + \left(r\rho_g K_{r,g} f_g\right)_P^{k+1}}{2}$$

$$\left(r\rho_g K_{r,g} f_g\right)_o^{k+1} = \frac{\left(r\rho_g K_{r,g} f_g\right)_O^{k+1} + \left(r\rho_g K_{r,g} f_g\right)_P^{k+1}}{2}$$

And :

$$\int_{k}^{k+1} \frac{gK_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{r}}\left(r{\rho_g}^2 K_{r,g}\right) drdzdt = \frac{gK_{ig}}{\mu_g}\left(\left(r{\rho_g}^2 K_{r,g}\right)_e^{k+1} - \left(r{\rho_g}^2 K_{r,g}\right)_o^{k+1}\right)\Delta z \Delta t = \frac{gK_{ig}}{2\mu_g}\left(\left(r{\rho_g}^2 K_{r,g}\right)_E^{k+1} - \left(r{\rho_g}^2 K_{r,g}\right)_O^{k+1}\right)\Delta z \Delta t$$

And :

$$\left(r{\rho_g}^2 K_{r,g}\right)_e^{k+1} = \frac{\left(r{\rho_g}^2 K_{r,g}\right)_E^{k+1} + \left(r{\rho_g}^2 K_{r,g}\right)_P^{k+1}}{2}$$

$$\left(r{\rho_g}^2 K_{r,g}\right)_o^{k+1} = \frac{\left(r{\rho_g}^2 K_{r,g}\right)_O^{k+1} + \left(r{\rho_g}^2 K_{r,g}\right)_P^{k+1}}{2}$$

Also :

$$\int_{k}^{k+1} \frac{K_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{z}}\left(\rho_g K_{r,g} f_g\right) rdrdzdt = \frac{K_{ig}}{\mu_g} r_p \left(\left(\rho_g K_{r,g} f_g\right)_n^{k+1} - \left(\rho_g K_{r,g} f_g\right)_s^{k+1}\right)\Delta r \Delta t = \frac{K_{ig}}{2\mu_g} r_p \left({\rho_g}_N^{k+1}\left(K_{r,g} f_g\right)_N^{k+1} - {\rho_g}_S^{k+1}\left(K_{r,g} f_g\right)_S^{k+1}\right)\Delta r \Delta t$$

And :

$$\int_{k}^{k+1}\frac{gK_{ig}}{\mu_g}\frac{\partial}{\partial \mathrm{z}}({\rho_g}^2K_{r,g})rdrdzdt=\frac{gK_{ig}}{\mu_g}r_p\left(\left({\rho_g}^2K_{r,g}\right)_n^{k+1}-\left({\rho_g}^2K_{r,g}\right)_s^{k+1}\right)\Delta r\Delta t$$
$$=\frac{gK_{ig}}{2\mu_g}r_p\left(\left({\rho_g}^2K_{r,g}\right)_N^{k+1}-\left({\rho_g}^2K_{r,g}\right)_S^{k+1}\right)\Delta r\Delta t$$

Finally we got the following :

$$\begin{aligned}
n\left(1-{S_l}_p^k\right)\left({\rho_g}_p^{k+1}-{\rho_g}_p^k\right)r_p\Delta r\Delta z-{\rho_g}_p^kW_p^{k+1}r_p\Delta r\Delta z\Delta t&\\
-\frac{K_{ig}}{2\mu_g}r_p\left({\rho_g}_N^{k+1}\left(K_{r,g}f_g\right)_N^{k+1}-{\rho_g}_S^{k+1}\left(K_{r,g}f_g\right)_S^{k+1}\right)\Delta r\Delta t&\\
-\frac{K_{ig}}{2\mu_g}\left(\left(\rho_g\right)_E^{k+1}\left(rK_{r,g}f_g\right)_E^{k+1}-\left(\rho_g\right)_O^{k+1}\left(rK_{r,g}f_g\right)_O^{k+1}\right)\Delta z\Delta t&\\
=\alpha{_g}_p^{k+1}r_p\Delta r\Delta z\Delta t-\frac{gK_{ig}}{2\mu_g}r_p\left(\left({\rho_g}^2K_{r,g}\right)_N^{k+1}-\left({\rho_g}^2K_{r,g}\right)_S^{k+1}\right)\Delta r\Delta t&\\
-\frac{gK_{ig}}{2\mu_g}\left(\left(r{\rho_g}^2K_{r,g}\right)_E^{k+1}-\left(r{\rho_g}^2K_{r,g}\right)_O^{k+1}\right)\Delta z\Delta t&
\end{aligned}$$

3.2 Energy conservation

By integrating equation (III) following the control volume (rdrdz) and along the time interval of length dt, it comes:

$$\iiint_t^{dt+t}\left(\rho C_p\right)^*\frac{\partial T}{\partial t}rdtdrdz+\iiint_t^{dt+t}\left(\rho C_p\right)_f\left(U_{p1}\frac{\partial T}{\partial r}+U_{p2}\frac{\partial T}{\partial z}\right)rdtdrdz$$
$$=\iiint_t^{dt+t}\frac{\lambda^*}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)rdtdrdz+\iiint_t^{dt+t}\lambda^*\frac{\partial^2T}{\partial z^2}rdtdrdz$$
$$+\iiint_t^{dt+t}Q\,rdtdrdz$$

By calculating term by term the integrals of the above equation, we find:

$$\iiint_t^{dt+t}\left(\rho C_p\right)^*\frac{\partial T}{\partial t}rdtdrdz=\mathrm{r_p}\left(\rho C_p\right)^*\left(T_p^{dt+t}-T_p^t\right)\Delta r\Delta z$$

And :

$$\iiint_t^{dt+t}\left(\rho C_p\right)_f\left(U_{p1}\frac{\partial T}{\partial r}\right)rdtdrdz=\mathrm{r_p}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}[T_e^{dt+t}-T_o^{dt+t}]\Delta t\Delta z$$
$$=\mathrm{r_p}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}[T_E^{dt+t}-T_O^{dt+t}]\frac{\Delta t\Delta z}{2}$$

$$\iiint_t^{dt+t} (\rho C_p)_f \left(U_{p2}\frac{\partial T}{\partial z}\right) rdtdrdz = \mathrm{r_p}(\rho C_p)_f (U_{p2})_p^{k+1}[T_n^{dt+t} - T_s^{dt+t}]\Delta t\Delta r$$

$$= \mathrm{r_p}(\rho C_p)_f (U_{p2})_p^{k+1}[T_N^{dt+t} - T_S^{dt+t}]\frac{\Delta t\Delta r}{2}$$

With :

$$T_e^{dt+t} = \frac{T_E^{dt+t} + T_p^{dt+t}}{2}$$

$$T_o^{dt+t} = \frac{T_p^{dt+t} + T_O^{dt+t}}{2}$$

$$T_n^{dt+t} = \frac{T_N^{dt+t} + T_p^{dt+t}}{2}$$

$$T_s^{dt+t} = \frac{T_P^{dt+t} + T_S^{dt+t}}{2}$$

$$\iiint_t^{dt+t} \lambda^* \frac{\partial^2 T}{\partial z^2} rdtdrdz = \lambda^* \mathrm{r_p}\left[\left(\frac{\partial T}{\partial z}\right)_{\mathrm{n}}^{\mathrm{dt+t}} - \left(\frac{\partial T}{\partial z}\right)_{\mathrm{s}}^{\mathrm{dt+t}}\right]\Delta \mathrm{r}\Delta \mathrm{t}$$

$$= \lambda^* \mathrm{r_p}\frac{\Delta\mathrm{r}\Delta\mathrm{t}}{\Delta z}[T_N^{dt+t} + T_S^{dt+t} - 2T_p^{dt+t}]$$

With :

$$\left(\frac{\partial T}{\partial z}\right)_{\mathrm{n}}^{\mathrm{dt+t}} = \frac{T_N^{dt+t} - T_p^{dt+t}}{\Delta z}$$

$$\left(\frac{\partial T}{\partial z}\right)_{\mathrm{s}}^{\mathrm{dt+t}} = \frac{T_P^{dt+t} - T_S^{dt+t}}{\Delta z}$$

$$\iiint_t^{dt+t} \lambda^* \frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) dtdrdz = \lambda^*\left[\mathrm{r_e}\left(\frac{\partial T}{\partial r}\right)_e^{dt+t} - \mathrm{r_o}\left(\frac{\partial T}{\partial r}\right)_o^{dt+t}\right]\Delta z\Delta t$$

$$= \lambda^* \frac{\Delta z\Delta t}{\Delta r}[\mathrm{r_e}T_E^{dt+t} + \mathrm{r_o}T_O^{dt+t} - (\mathrm{r_o} + \mathrm{r_e})T_p^{dt+t}]$$

With :

$$\mathrm{r_e} = \frac{\mathrm{r_E} + \mathrm{r_P}}{2}$$

$$\mathrm{r_o} = \frac{\mathrm{r_O} + \mathrm{r_P}}{2}$$

$$\left(\frac{\partial T}{\partial r}\right)_e^{dt+t} = \frac{T_E^{dt+t} - T_p^{dt+t}}{\Delta r}$$

$$\left(\frac{\partial T}{\partial r}\right)_o^{dt+t} = \frac{T_P^{dt+t} - T_O^{dt+t}}{\Delta r}$$

$$\iiint_{t}^{dt+t} Q\, rdtdrdz = Qr_p\Delta r\Delta z\Delta t$$

Where :

$$\left(\mathrm{r_P}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}-\frac{\lambda^*\mathrm{r_e}}{\Delta r}\right)\Delta z\Delta t T_E^{dt+t}-\left(\mathrm{r_P}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}+\frac{\lambda^*\mathrm{r_o}}{\Delta r}\right)\Delta z\Delta t T_O^{dt+t}$$
$$+\mathrm{r_p}\Delta t\Delta r\left(\left(\rho C_p\right)_f\frac{\left(U_{p2}\right)_p^{k+1}}{2}-\frac{\lambda^*}{\Delta z}\right)T_N^{dt+t}-\mathrm{r_p}\Delta t\Delta r\left(\left(\rho C_p\right)_f\frac{\left(U_{p2}\right)_p^{k+1}}{2}+\frac{\lambda^*}{\Delta z}\right)T_S^{dt+t}$$
$$+\left[\mathrm{r_p}\left(\rho C_p\right)^*\Delta r\Delta z+\lambda^*(\mathrm{r_o}+\mathrm{r_e})\frac{\Delta \mathrm{z}\Delta \mathrm{t}}{\Delta r}+2\lambda^*\mathrm{r_p}\frac{\Delta \mathrm{r}\Delta \mathrm{t}}{\Delta z}\right]T_p^{dt+t}=\mathrm{r_p}\left(\rho C_p\right)^*\Delta r\Delta z T_p^t+Qr_p\Delta r\Delta z\Delta t$$

The equation can therefore be put in the following form:

$$\mathrm{A(i,j)T_{(i+1,j)}^{dt+t}}+\mathrm{B(i,j)T_{(i,j+1)}^{dt+t}}+\mathrm{C(i,j)T_{(i-1,j)}^{dt+t}}+\mathrm{F(i,j)T_{(i,j)}^{dt+t}}+\mathrm{G(i,j)T_{(i,j-1)}^{dt+t}}=\mathrm{D(i,j)} \qquad (6)$$

With :

$$\mathrm{A(i,j)}=\left(\mathrm{r_P}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}-\frac{\lambda^*(2\mathrm{r_P}+\Delta r)}{2\Delta r}\right)\Delta z\Delta t$$

$$\mathrm{B(i,j)}=\mathrm{r_p}\Delta t\Delta r\left(\left(\rho C_p\right)_f\frac{\left(U_{p2}\right)_p^{k+1}}{2}-\frac{\lambda^*}{\Delta z}\right)$$

$$\mathrm{C(i,j)}=-\left(\mathrm{r_P}\left(\rho C_p\right)_f\left(U_{p1}\right)_p^{k+1}+\frac{\lambda^*(2\mathrm{r_P}-\Delta r)}{2\Delta r}\right)\Delta z\Delta t$$

$$\mathrm{F(i,j)}=\mathrm{r_p}\left(\rho C_p\right)^*\Delta r\Delta z+\lambda^*\mathrm{r_p}\frac{\Delta \mathrm{z}\Delta \mathrm{t}}{2\Delta r}+2\lambda^*\mathrm{r_p}\frac{\Delta \mathrm{r}\Delta \mathrm{t}}{\Delta z}$$

$$\mathrm{G(i,j)}=-\mathrm{r_p}\Delta t\Delta r\left(\left(\rho C_p\right)_f\frac{\left(U_{p2}\right)_p^{k+1}}{2}+\frac{\lambda^*}{\Delta z}\right)$$

$$\mathrm{D(i,j)}=\mathrm{r_p}\left(\rho C_p\right)^*\Delta r\Delta z T_p^t+Qr_p\Delta r\Delta z\Delta t$$

3.3 The equations of biogas production

3.3.1 Runge-Kutta methods

Carl Runge (1856-1927) and Martin Kutta (1867-1944) proposed in 1895 to solve the Cauchy problem. The Runge-Kutta methods have the advantage of having higher and higher orders while avoiding the computation of the derivatives required for the Taylor methods.

$$\begin{cases}\dfrac{\partial y}{\partial t}=f(y,t)\\ y(t=0)=y_0\end{cases}$$

According to the Runge-Kutta 2nd order method this equation is written:

$$Y^{k+1}(i,j)=Y^k(i,j)+\Delta t f\left(Y^{k+\frac{1}{2}}(i.j)\right)$$

$$Y^{k+1/2}(i,j) = Y^k(i,j) + \frac{\Delta t}{2} f\left(Y^k(i.j)\right)$$

We discretize the different equations of biogas production by the Runge-Kutta 2nd order method.

3.3.2 ADM1 Model: Runge-Kutta 2nd order method discretization

We discretize the deferent equations of biogas production by the Runge-Kutta 2nd order method.

- The equation of the concentration of sugars becomes:

$$\frac{dS_{su}}{dt} = f(S_{su})$$

With:

$$f(S_{su}) = -k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su} + S_{su}}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{su}{}^{k+1} = S_{su}{}^{k} + \Delta t \times f\left(S_{su}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{su}{}^{k+\frac{1}{2}} = S_{su}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{su}{}^{k}\right)$$

With:

$$f\left(S_{su}{}^{k+\frac{1}{2}}\right) = -k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k+\frac{1}{2}}}{K_{s,su} + S_{su}{}^{k+\frac{1}{2}}}$$

And:

$$f\left(S_{su}{}^{k}\right) = -k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k}}{K_{s,su} + S_{su}{}^{k}}$$

- The equation of the concentration of butyrate becomes:

$$\frac{dS_{bu}}{dt} = f(S_{bu})$$

With:

$$f(S_{bu}) = (1 - Y_{Su}) \times f_{bu,su} \times k_{m,su} \times \frac{S_{su}}{K_{s,su} + S_{su}} \times X_{su} - k_{m,c4} \times \frac{S_{bu}}{K_{s,c4} + S_{bu}} \times X_{c4} \times \frac{1}{1 + \frac{S_{va}}{S_{bu}}}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{bu}{}^{k+1} = S_{bu}{}^{k} + \Delta t \times f\left(S_{bu}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{bu}{}^{k+\frac{1}{2}} = S_{bu}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{bu}{}^{k}\right)$$

With:

$$f\left(S_{bu}{}^{k+\frac{1}{2}}\right) = (1 - Y_{Su}) \times f_{bu,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k+\frac{1}{2}}}{K_{s,su} + S_{su}{}^{k+\frac{1}{2}}} - k_{m,c4} \times X_{c4} \times \frac{S_{bu}{}^{k+\frac{1}{2}}}{K_{s,c4} + S_{bu}{}^{k+\frac{1}{2}}}$$

And:

$$f\left(S_{bu}{}^{k}\right) = (1 - Y_{Su}) \times f_{bu,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k}}{K_{s,su} + S_{su}{}^{k}} - k_{m,c4} \times X_{c4} \times \frac{S_{bu}{}^{k}}{K_{s,c4} + S_{bu}{}^{k}}$$

- The equation of the concentration of propionate becomes:

$$\frac{dS_{pro}}{dt} = f\left(S_{pro}\right)$$

With:

$$f\left(S_{pro}\right) = (1 - Y_{Su}) \times f_{pro,su} \times k_{m,su} \frac{S_{su}}{K_{s,su} + S_{su}} \times X_{su} - k_{m,pro} \times \frac{S_{pro}}{K_{s,pro} + S_{pro}} \times X_{pro}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{pro}{}^{k+1} = S_{pro}{}^{k} + \Delta t \times f\left(S_{pro}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{pro}{}^{k+\frac{1}{2}} = S_{pro}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{pro}{}^{k}\right)$$

With:

$$f\left(S_{pro}{}^{k+\frac{1}{2}}\right) = (1 - Y_{Su}) \times f_{pro,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k+\frac{1}{2}}}{K_{s,su} + S_{su}{}^{k+\frac{1}{2}}} - k_{m,pro} \times X_{pro} \times \frac{S_{pro}{}^{k+\frac{1}{2}}}{K_{s,pro} + S_{pro}{}^{k+\frac{1}{2}}}$$

And:

$$f\left(S_{pro}{}^{k}\right) = (1 - Y_{Su}) \times f_{pro,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k}}{K_{s,su} + S_{su}{}^{k}} - k_{m,pro} \times X_{pro} \times \frac{S_{pro}{}^{k}}{K_{s,pro} + S_{pro}{}^{k}}$$

- The equation of the concentration of acetate becomes:

$$\frac{dS_{ac}}{dt} = f\left(S_{ac}\right)$$

With:

$$f(S_{ac}) = (1 - Y_{Su}) \times f_{ac,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}}{K_{s,su} + S_{su}} + (1 - Y_{c4}) \times 0{,}8 \times k_{m,c4} \times X_{c4} \times \frac{S_{bu}}{K_{s,c4} + S_{bu}} + \left(1 - Y_{pro}\right) \times 0{,}57 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}}{K_{s,pro} + S_{pro}} - k_{m,ac} \times X_{ac} \times \frac{S_{ac}}{K_{s,ac} + S_{ac}}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{ac}{}^{k+1} = S_{ac}{}^{k} + \Delta t \times f\left(S_{ac}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{ac}{}^{k+\frac{1}{2}} = S_{ac}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{ac}{}^{k}\right)$$

With:

$$f\left(S_{ac}{}^{k+\frac{1}{2}}\right) = (1 - Y_{Su}) \times f_{ac,su} \times k_{m,su} \times \frac{S_{su}{}^{k+\frac{1}{2}}}{K_{s,su} + S_{su}{}^{k+\frac{1}{2}}} \times X_{su} + (1 - Y_{c4}) \times 0{,}8 \times k_{m,c4} \times X_{c4} \times \frac{S_{bu}{}^{k+\frac{1}{2}}}{K_{s,c4} + S_{bu}{}^{k+\frac{1}{2}}} + \left(1 - Y_{pro}\right) \times 0{,}57 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}{}^{k+\frac{1}{2}}}{K_{s,pro} + S_{pro}{}^{k+\frac{1}{2}}} - k_{m,ac} \times X_{ac} \times \frac{S_{ac}{}^{k+\frac{1}{2}}}{K_{s,ac} + S_{ac}{}^{k+\frac{1}{2}}}$$

And:

$$f\left(S_{ac}{}^{k}\right) = (1 - Y_{Su}) \times f_{ac,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k}}{K_{s,su} + S_{su}{}^{k}} + (1 - Y_{c4}) \times 0{,}8 \times k_{m,c4} \times X_{c4} \times \frac{S_{bu}{}^{k}}{K_{s,c4} + S_{bu}{}^{k}} + \left(1 - Y_{pro}\right) \times 0{,}57 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}{}^{k}}{K_{s,pro} + S_{pro}{}^{k}} - k_{m,ac} \times X_{ac} \times \frac{S_{ac}{}^{k}}{K_{s,ac} + S_{ac}{}^{k}}$$

- The equation of the concentration of hydrogen becomes:

$$\frac{dS_{H2}}{dt} = f(S_{H2})$$

With

$$f(S_{H2}) = (1 - Y_{Su}) \times f_{H2,su} \times k_{m,su} \times \frac{S_{su}}{K_{s,su} + S_{su}} \times X_{su} + (1 - Y_{c4}) \times 0{,}2 \times k_{m,c4} \times \frac{S_{bu}}{K_{s,c4} + S_{bu}} \times X_{c4} \times \frac{1}{1 + \frac{S_{va}}{S_{bu}}} + \left(1 - Y_{pro}\right) \times 0{,}43 \times k_{m,pro} \times \frac{S_{pro}}{K_{s,pro} + S_{pro}} \times X_{pro} - k_{m,H2} \times \frac{S_{H2}}{K_{s,H2} + S_{H2}} \times X_{H2}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{H2}{}^{k+1} = S_{H2}{}^{k} + \Delta t \times f\left(S_{H2}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{H2}{}^{k+\frac{1}{2}} = S_{H2}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{H2}{}^{k}\right)$$

With:

$$f\left(S_{H2}{}^{k+\frac{1}{2}}\right) = (1 - Y_{Su}) \times f_{H2,su} \times k_{m,su} \times X_{su} \times \frac{S_{su}{}^{k+\frac{1}{2}}}{K_{s,su} + S_{su}{}^{k+\frac{1}{2}}} + (1 - Y_{c4}) \times 0{,}2 \times k_{m,c4} \times X_{c4} \times \frac{S_{bu}{}^{k+\frac{1}{2}}}{K_{s,c4} + S_{bu}{}^{k+\frac{1}{2}}} + \left(1 - Y_{pro}\right) \times 0{,}43 \times k_{m,pro} \times X_{pro} \times \frac{S_{pro}{}^{k+\frac{1}{2}}}{K_{s,pro} + S_{pro}{}^{k+\frac{1}{2}}} - k_{m,H2} \times X_{H2} \times \frac{S_{H2}{}^{k+\frac{1}{2}}}{K_{s,H2} + S_{H2}{}^{k+\frac{1}{2}}}$$

And:

- The equation of the concentration of methane becomes:

$$\frac{dS_{ch4}}{dt} = f(S_{ch4})$$

With:

$$f(S_{ch4}) = (1 - Y_{ac}) \times k_{m,ac} \times \frac{S_{ac}}{K_{s,ac} + S_{ac}} \times X_{ac} + (1 - Y_{H2}) \times k_{m,H2} \times \frac{S_{H2}}{K_{s,H2} + S_{H2}} \times X_{H2}$$

According to Runge-Kutta 2nd order method, this equation is written:

$$S_{ch4}{}^{k+1} = S_{ch4}{}^{k} + \Delta t \times f\left(S_{ch4}{}^{k+\frac{1}{2}}\right)$$

Also:

$$S_{ch4}{}^{k+\frac{1}{2}} = S_{ch4}{}^{k} + \frac{\Delta t}{2} \times f\left(S_{ch4}{}^{k}\right)$$

With:

$$f\left(S_{ch4}{}^{k+\frac{1}{2}}\right) = (1 - Y_{ac}) \times k_{m,ac} \times X_{ac} \times \frac{S_{ac}{}^{k+\frac{1}{2}}}{K_{s,ac} + S_{ac}{}^{k+\frac{1}{2}}} + (1 - Y_{H2}) \times k_{m,H2} \times X_{H2} \times \frac{S_{H2}{}^{k+\frac{1}{2}}}{K_{s,H2} + S_{H2}{}^{k+\frac{1}{2}}}$$

And:

$$f\left(S_{ch4}{}^{k}\right) = (1 - Y_{ac}) \times k_{m,ac} \times X_{ac} \times \frac{S_{ac}{}^{k}}{K_{s,ac} + S_{ac}{}^{k}} + (1 - Y_{H2}) \times k_{m,H2} \times X_{H2} \times \frac{S_{H2}{}^{k}}{K_{s,H2} + S_{H2}{}^{k}}$$

• Conclusion

We obtained in the previous chapter a system of equations which do not admit analytical solutions where recourse to numerical methods turns out to be compulsory. We opted for the use of the finite volume method and the implicit Runge-Kutta method at order 2. All the equations are discretized according to a scheme centered in space and delayed in time.

The calculations are initiated using an initial profile which satisfies the boundary conditions. The use of these values allows the determination of the temperature profiles, the liquid saturation and the concentrations at each stage of the degradation. All the algebraic equations will be solved using a numerical code in FORTRAN and the results as well as their interpretations will be presented in the following chapter.

CHAPTER 5

RESULTS AND DISCUSSIONS

• 1. Introduction

We have made our Fortran program which allows us to simulate the ADM1 model with 35 state variables. This model of anaerobic digestion as mentioned above contains time scales with different dimensions and quite heterogeneous variables, which makes us believe that it belongs to the class of extremely sensitive stiff systems, therefore requiring a certain parameterization and a correct choice of solver!

In fact, simulate a nonlinear model with more than 130 parameters, at different time scales (variables quickly reaching their steady state, while others are slower), variables which must be positive because they are about biology, ... Is a job which is not easy and which is constrained by various bugs.

1.2 Simulating stiff systems

A system is called stiff, when the range of the time constants is large. This means that some of the system states react quickly whereas some react sluggishly. The ADM1 is a very stiff system with time constants ranging from fractions of a second to months. This makes the simulation of such a system challenging and in order to avoid excessively long simulation times, one needs to be somewhat creative when implementing the model.

1.3 ODE and DAE systems

When the states of a system are described only by ordinary differential equations, the system is said to be an ODE system. If the system is stiff, it is sometimes possible to rewrite some of the system equations in order to omit the fastest states. The rationale for this is that from the slower state's point of view, the fast states can be considered instantaneous and possible to describe by algebraic equations. Such systems are normally referred to as differential algebraic equation (DAE) systems. By rewriting an ODE system to a DAE system, the stiffness can be decreased, allowing for explicit solvers to be used and for stochastic elements to be incorporated. The drawback is that the DAE system is only an approximation of the original system and the effect of this approximation must be considered and investigated for each specific simulation model.

1.4 Time constants in ADM1

As mentioned before, the ADM1 includes time constants in a wide range; from milliseconds for pH to weeks or months for the states describing various fractions of active biomass. Since most control actions affecting the anaerobic digester are fairly slow, it makes sense to investigate which fast states can be approximated by algebraic equations. In Batstone et al. (2002), it is suggested that the pH (S_{H+}) state is calculated by algebraic equations. However, this will only partially solve the stiffness problem. There are other fast states and a closer investigation suggests that the state describing hydrogen (S_{h2}) also needs to be approximated by an algebraic equation.

2. Results and interpretations

In the Maize waste used in our simulation, we have considered that our residues have contained a big amount of carbohydrates, with small quantities of lipids and fat. Therefore, we have used sugar (glucose) as the key substrate in our organic waste. As many investigations from recent papers have shown the effect of pH parameter on the production of biogas (methane), as well our simulation shows significant rises in the CH_4 concentration. The highest value of methane concentration as has been observed in *Figure 16*, is when the pH is about 6.

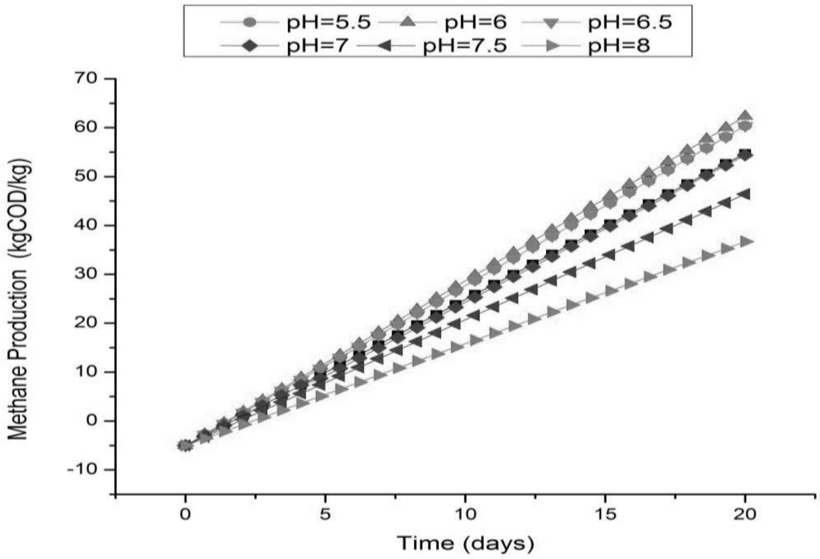

Figure 16: The effect of different initial pH on methane production

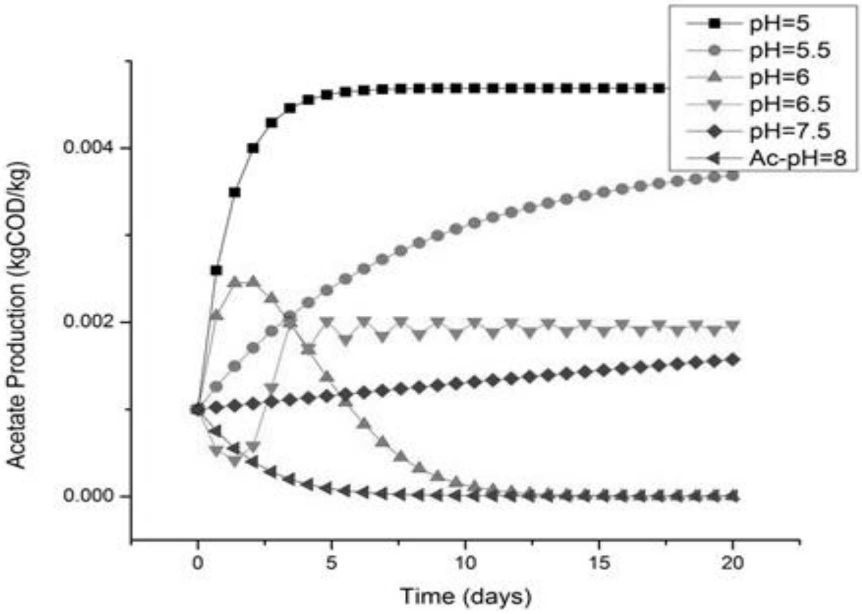

Figure 17: Production of acetate with different values of pH.

As a result of many investigations done behind the factors that influence on methane production, they have found that many criterions such as the initial pH value and temperature have an impact on the methanogenesis activity of bacteria (Fathepure B. Z. al, 1987).

It has evidenced that a rise of temperature and the initial pH value can directly lead to an increase in the biomethanization process by the impact of the hydrogen (H_2) concentration due to the hydrogen-producing bacteria.

The sharp decrease of acetate concentration due the impact of the phenomena of inhibition, as we can see from the *Figure 17*, we can say that acetate concentration is the most influential parameter by the inhibition caused by the propionate (Lee, Myung-Yeol al, 2009), especially from the value of (pH= 6), we observe that the concentration of acetate has decreased from that value of pH.

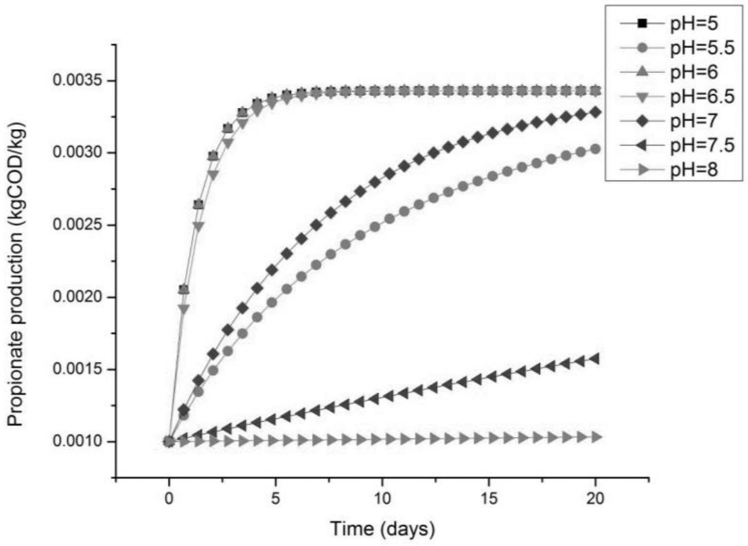

Figure 18: Production of propionate with different values of pH

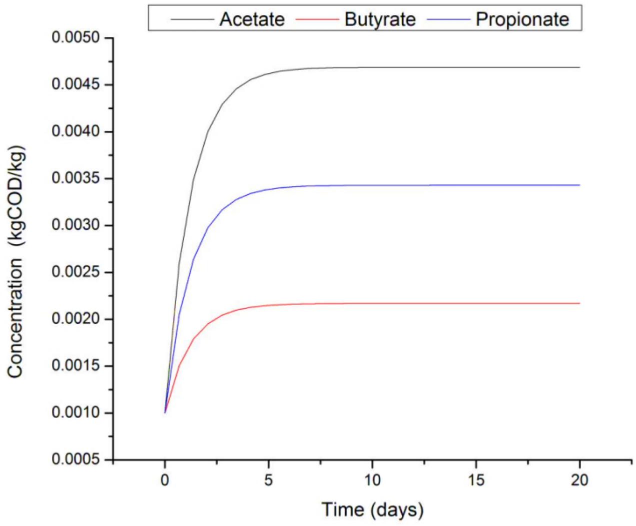

Figure 19: Production of volatile fatty acids

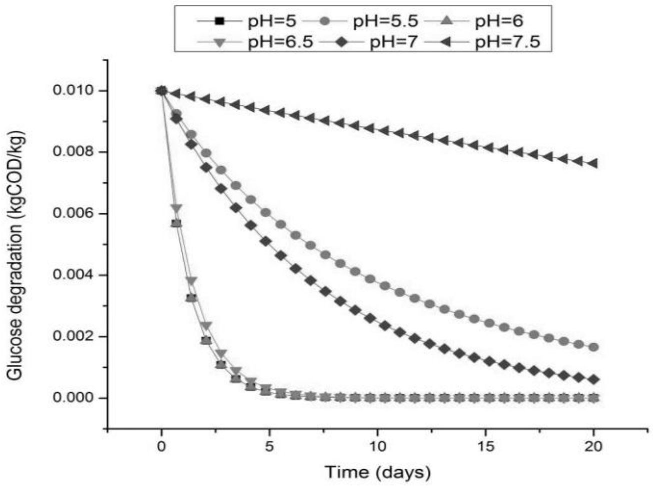

Figure 20: Concentration of glucose under different values of pH

The degradation of glucose concentrations has strongly decreased as we have witnessed in *Figure 20*, and this is because of the values of pH. The phenomena of inhibition have clearly impacted the concentration of the main substrate.

Analysis of sensitivity, *Figure 21*, showed that $K_{m.process}$ (maximum direct uptake rate) and $K_{S.process}$ (half saturation value) were highly sensitive to variable simulations (Ali, Zulfiqar et al,. 2014).

Essential parameters are calculated using iterative methods, including maximum uptake rate for propionate users ($k_{m,pro}$) and half saturation constant for acetate users ($K_{s,ac}$) in the thermophilic digester and maximum uptake rate for acetate users ($k_{m,ac}$) in the mesophilic digester, improving the parameters with experimental results (Anukam, A et al., 2019).

The values of the kinetics parameters such as the k_m which is the specific Monod maximum uptake rate has not an important influence, conversely, the Monod half-saturation for example of acetate $k_{s,ac}$ impact directly on the acetate concentration as well on the methane concentration.

The stoichiometric parameters such as the yield of the product on substrate $f_{product\ ,substrate}$ has shown high values of almost the whole components and finally the yield of biomass on the substrate $Y_{substrate}$ this parameter is not very important as many studies have shown (Ali, Zulfiqar et al,. 2014; Anukam, A et al., 2019).

The sensitivity of $k_{s,ac}$ and $k_m X_{ac}$ has shown a high influence on the of the kinetic of degradation and as a result, the production of biogas (methane) has increased once we have added a small variation of 10% on the parameter of $k_m X_{ac}$ as we keep the value of $k_{s,ac}$ fixe for the other simulations.

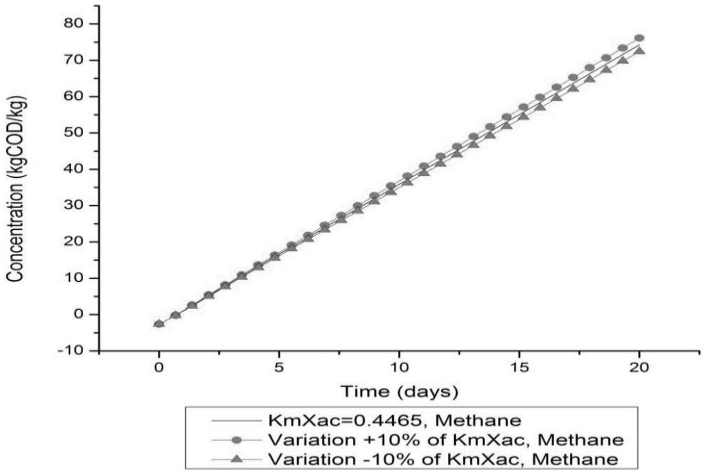

Figure 21: Influence of $km\ Xac$ on rate of methane production

In order to fit the model parameter that describes the evolution of the anaerobic process, it's recommended by Rosen and Jeppsson 2005 (Jeppsson, Ulf et al., 2005), to set the initial values as the first step of the model parameters, then simulating the model with those values and changing the most sensitive parameter such as the maximum Monod uptake rate of acetate, for example, $K_{m,ac}$, as well as the Monod half-saturation parameter of acetate $K_{s,ac}$, until finding the best values of those parameters.

Some parameters are still in their original form as they come from the paper of Batstone 2002 (D.J. Batstone et al., 2002), without any modification applied to them because of its poor influence on the optimization of the model.

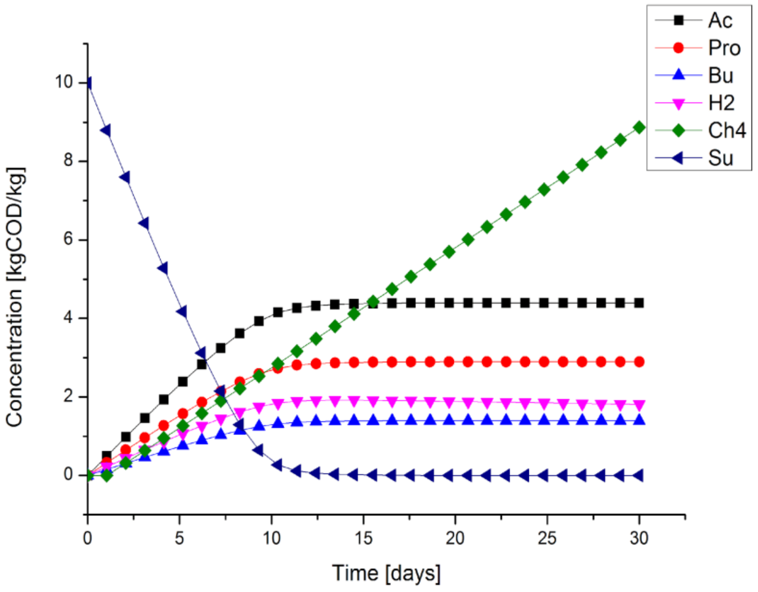

Figure 22: Simulation results of anaerobic glucose degradation

The results obtained from the simulation of ODEs have been shown in *Figure 22*. As seen from the graph there's a slight decrease of glucose (S_{Su}) with the sharp increase of methane (S_{CH4}), while the production of volatile fatty acids (S_{ac}, S_{Pro}, S_{Bu}) simultaneously. Acetate being the last intermediate substrate for anaerobic digestion before the formation of methane, the influence of its degradation kinetics on biogas production is direct.

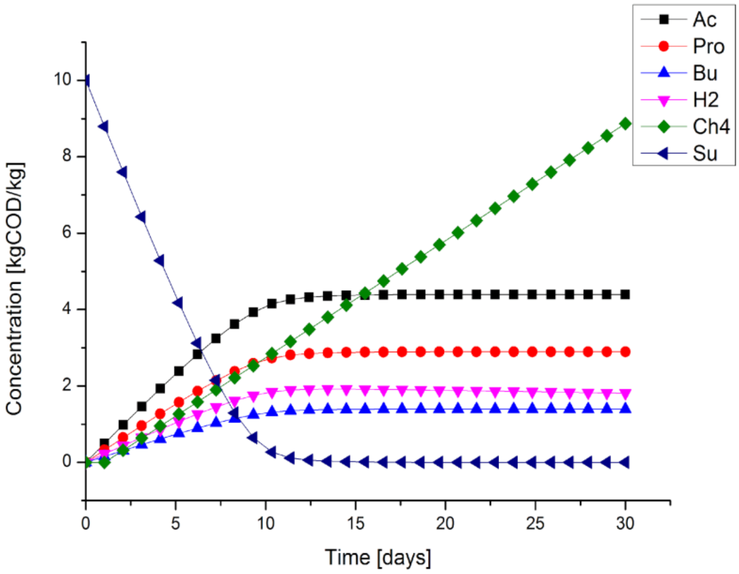

Figure 23: Effect of k_{La} on methane production

The mass transfer coefficient (k_{La}) is the most important factor when simulating transfers between the liquid phase and the gas phase. Although this parameter is extremely difficult to determine experimentally in anaerobic digestion plants (mainly because of the heterogeneity as well as the technical difficulty of this measurement in such an environment), taking it into account is decisive for the optimal functioning of the model. *Figure 23* illustrates the influence of k_{La} on methane production, as the kinetics of methane production by methanogens is similar in all cases. The influence of k_{La} on the kinetics of biogas production will be more clearly visible. The values of K_mX_{ac} and $K_{s,ac}$ retained (arbitrarily) for the study are 376 mgCOD.kg^{-1}. d^{-1} and 440 mgCOD.kg^{-1} respectively.

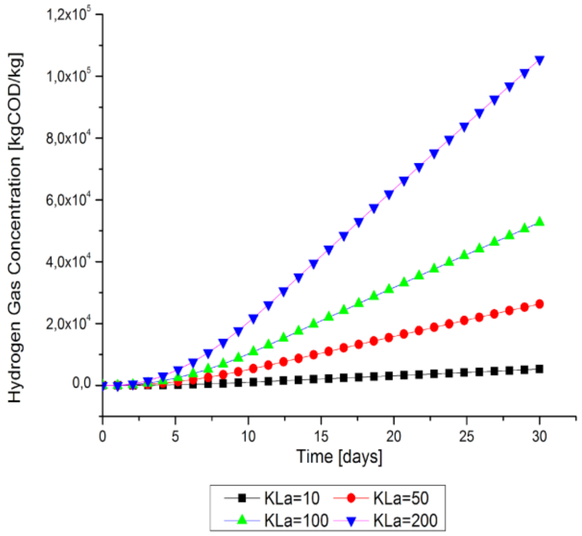

Figure 24: Effect of k_{La} on hydrogen production

As seen from *Figure 24* k_{La} has a big influence on the concentration of hydrogen ($S_{gas,H2}$), this effect explains the importance of this parameter on the methanogenic activity of bacteria.

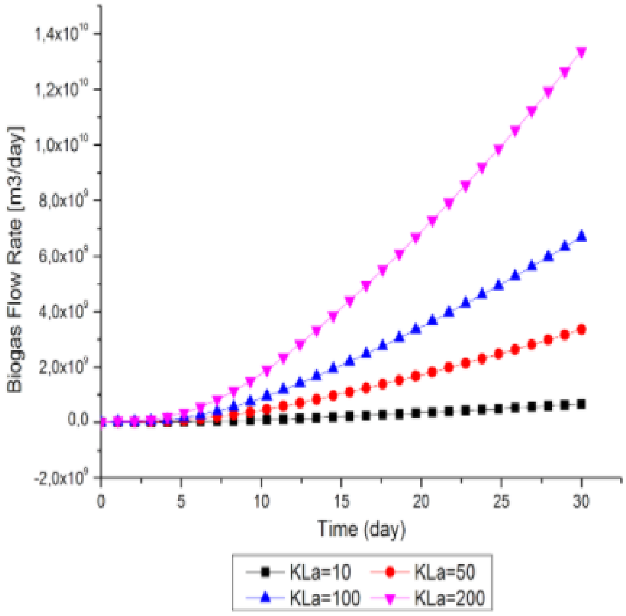

Figure 25: Effect of k_{La} on the biogas flow rate

The effect of k_{La} on the flow rate of biogas is clear from *Figure 25*. Thus, the parameter k_{La} influences the biogas production which in turn affects the flow rate.

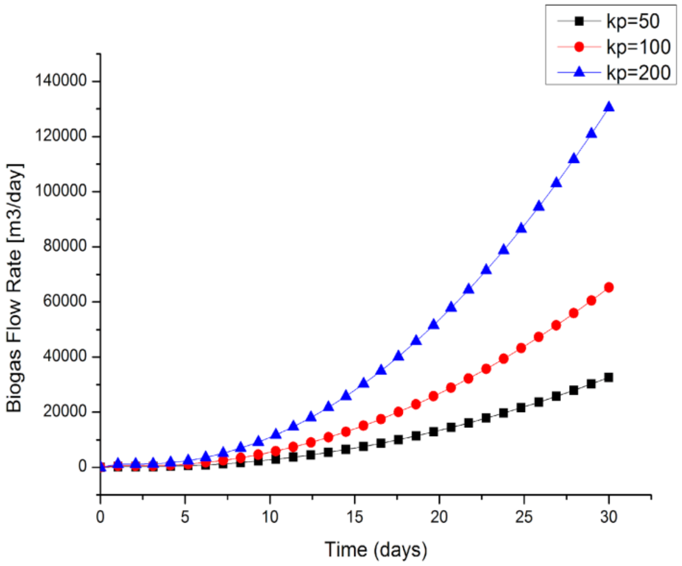

Figure 26: Effect of k_p on the biogas flow rate

The *Figure 26* shows the influence of the parameter k_p which is related to the friction of biogas in the gas outlet, this parameter plays the role of the correlation factor between the reactor pressure and the gas flow rate which has a unique effect on the model.

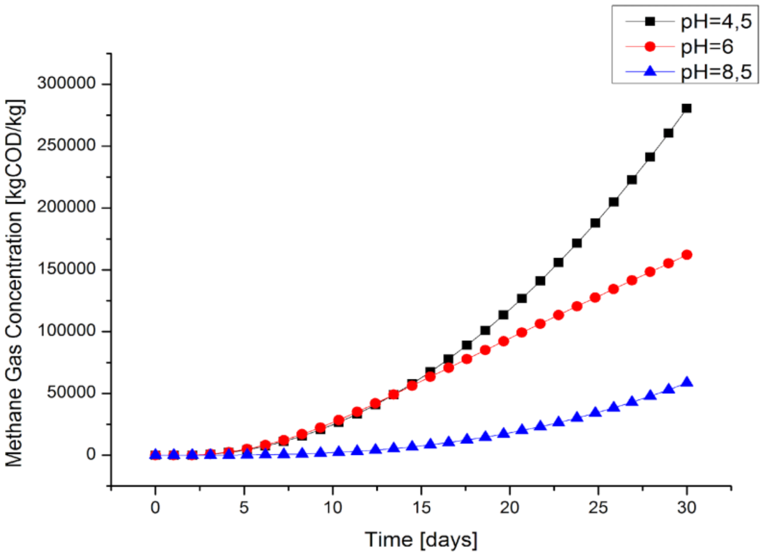

Figure 27: Methane production under different ranges of pH

Many recent studies have shown how pH can play a major effect on methanogenesis bacteria activity.

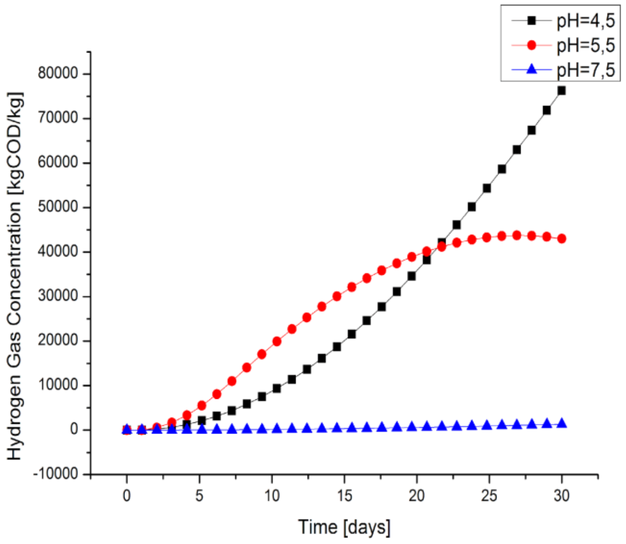

Figure 28: Hydrogen production under different ranges of pH

As well, the results obtained from the simulation of gas-phase equations under different ranges of pH shows that at the value (pH=4,5) the concentration of hydrogen has increased.

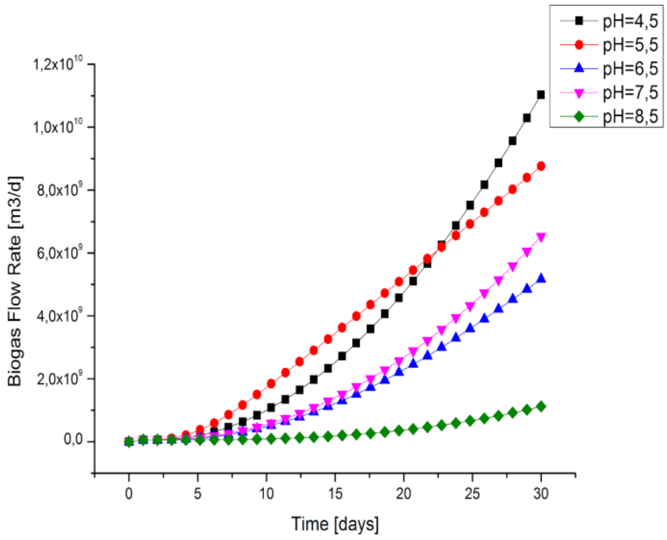

Figure 29: Biogas flow rate under different ranges of pH

Since the pH has the potential to shift the production of biogas, it can also impact the flow rate of biogas. As seen from the *Figure 29*, between the values of pH 4,5 and 5,5 the biogas flow rate has a slight increase with a slow increase when pH is upper than 6,5.

These results give us an idea how the reduction of waste was introduced, which results in a decrease in the production profile of biogas. Similar results have been found by other authors in the same topic of waste valorisation (Fezzani, Boubaker et al., 2004; Samir Men-La-Yakhaf et al., 2015; Belgada, R. et al., 2020).

As the *Figure 16* and *Figure 20* shown, the evolution of biogas mainly the methane production is inversely proportional with the decrease of glucose substances.
Finally, these results could be interpreted as the decrease of organic matter of maize residues which affects the production of methane gas as the main product of this investigation (Samir Men-La-Yakhaf et al., 2015; Belgada, R. et al., 2020; Mohcine, A et al., 2018).

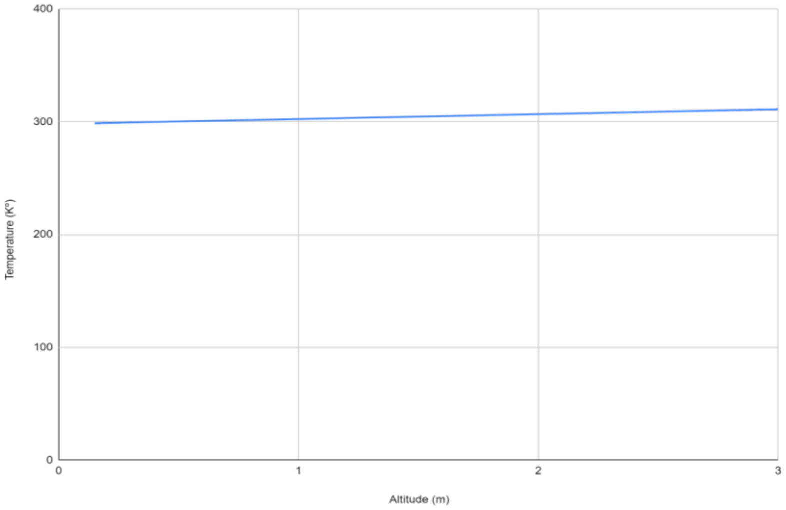

Figure 30: Influence of temperature on the axiale variable

Figure 30 illustrates the variation in temperature as a function of the axial variable. It can be seen that the temperature increases over time. This can be explained by the fact that over time the component settles and therefore the interactions between them increase and hence the temperature. We also notice that the temperature is a decreasing function according to the radial variable. This result can be interpreted by the fact that the maximum temperature on the pipe axis as well as it decreases going towards the wall to reach the value imposed on it. This result is qualitatively similar to those obtained by other authors working under similar conditions (Noble, J.J et al., 1991, Gil Diaz J et al., 1995; Van Genuchten M et al., 1991; Van Genuchten M al, 1980).

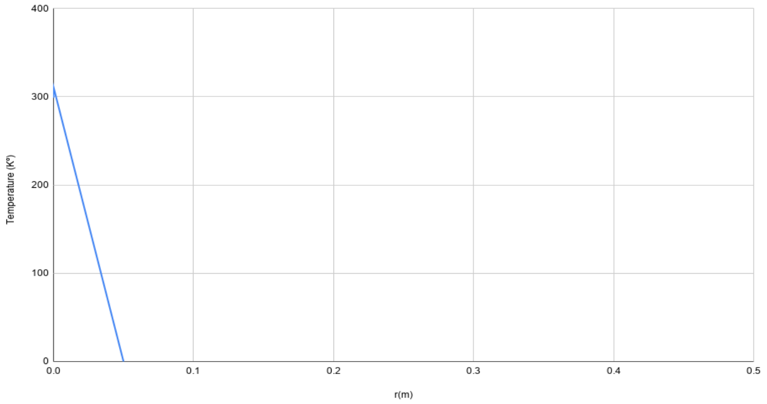

Figure 31: Influence of temperature on the radiale variable

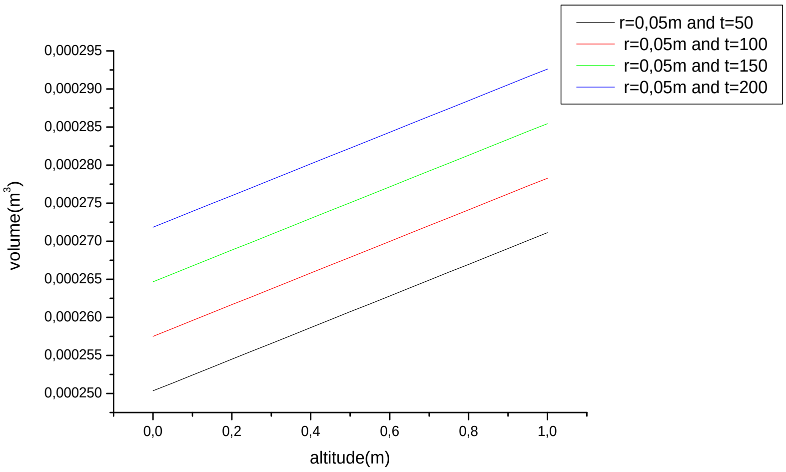

Figure 32: Saturation profile as a function of time and of the axial variable, and of the radial variable

Figure 33 shows the variation in saturation as a function of the axial variable. Note that this quantity increases slowly with this variable, quite logical, since the saturation increases from its minimum value and increases to reach the residual saturation of the medium. We also notice that the saturation is almost constant as a function of the radial variable. We obtain qualitatively similar results to those obtained by other (Samir Men-La-Yakhaf et al., 2015; Belgada, R. et al., 2020; Mohcine, A et al., 2018).

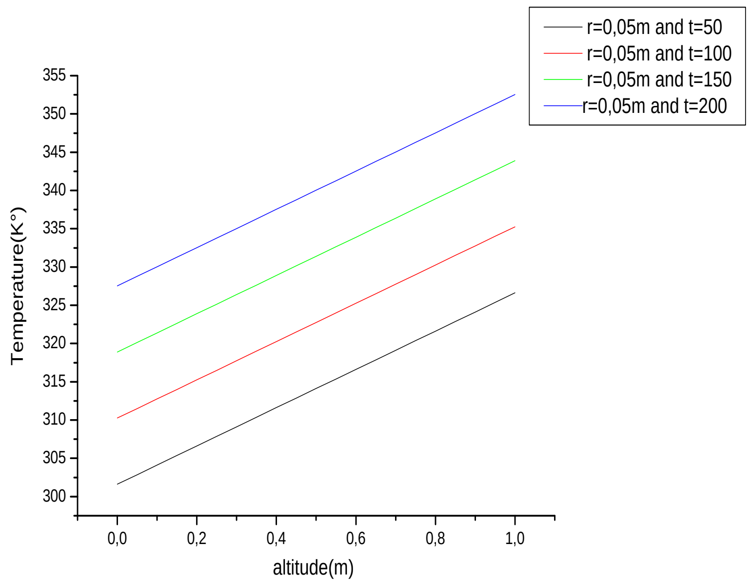

Figure 33: Temperature profile as a function of time, of the axial variable and of the radial variable

Figure 34 illustrates the temperature variation as a function of the axial variable. It can be seen that the temperature increases over time. This can be explained by the fact that over time the component is deposited, and therefore the interaction between them and therefore increases the temperature. We also notice that the temperature is a decreasing function according to the radial variable. This result can be interpreted by the fact that the maximum temperature on the pipe axis and decreases going towards the wall to reach the value imposed on it. This result is qualitatively similar to those obtained by other authors working under similar conditions (Samir Men-La-Yakhaf et al., 2015; Belgada, R. et al., 2020; Mohcine, A et al., 2018).

- ## Conclusion

In this chapter we presented the hydraulic and biological results of the numerical simulations using the ADM1 model coupled with the hydro-thermal model for the waste of maize. It can be seen that this mathematical model is considered the role of methanogenic biomass in the production of gas and heat. Also we've seen the most important parameters that influence the ADM1 model.

- # GENERAL CONCLUSION

Overexploited natural resources and an extremely polluted environment are the sad repercussions of the industrial development of the world. Faced with this critical situation, there is an urgent need to establish more rational policies, healthy enough to preserve our planet. In this sense, the treatment of wastewater and waste before discharging them into receiving environments has become an obligation.

In fact, "decontaminated" wastewater represents an alternative resource to conventional water, which can be reused in industry and agriculture. This is a real paradigm shift: reduce pollution and reuse treated water.

In this thesis we have examined the role of key parameters and processes of waste degradation and methane production in the anaerobic methanogenic phase, such as water content, temperature, waste density and leachate injection. The humidity of the waste is a determining factor in the degradation kinetics and therefore in gas production.

Some previous work shows that temperature is one of the most important parameters for anaerobic degradation and stabilization of waste. Despite the importance of temperature and its influence on various physical, biological and hydraulic aspects of waste and bioreactors, studies concerning this parameter are very limited. Thus, we have insisted in our work on the role of temperature and tried to explain the biological phenomena linked to microbial activity, as a function of temperature, as well as saturation. We have developed a numerical simulation model of hydraulic phenomena and two-phase flow of liquid and gas in bioreactors, in a first step.

In a second step, we presented different sensitivity analysis of the biological model and biogas production model, also the ADM1 model is coupled with the two-phase flow model, the modified model of ADM1 was based only on the microbial growth model of Monod (1949) and considers the role of methanogenic biomass in the production of gas and heat.

In this study, in order to demonstrate and evaluate the performance of ADM1, the anaerobic model for glucose degradation in a batch-type bottle reactor was constructed based on ADM1, and the sensitivities of kinetic and stoichiometric parameters to simulation results were analyzed.

Among five component concentrations, only methane concentration, which was found most to be sensitive on almost all the parameters, was used for optimization. However, $k_{m,ac}$ and X_{ac} were not successfully estimated. Combinations of $k_{m,ac}$ and X_{ac}, which had different values, showed a good accuracy in methane production and acetate degradation. It was thought that the linear relationship between $k_{m,ac}$ and X_{ac} makes them difficult to be estimated successfully. However, the values of $k_{m,ac} \cdot X_{ac}$ were almost identical, suggesting that it was more effective to estimate the combination of k and X for each process.

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