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MATHEMATICAL STUDY OF AN ANAEROBIC DIGESTION MODEL, PART 1

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Abstract. We will start by studying in great detail the simplest possible model that we will call "minimal model". It is minimal in the sense that if we tried to simplify it still a little, nothing would remain of what characterizes a "real" Chemostat. For this minimal model we assume that $s \Rightarrow (s)$ is a function of the substrate only and that the yield y(.) = Y is constant. We will engage in a very precise mathematical study of this model. It is not very difficult but it is imperative to understand all the details well because all the later studies, more complex, are based on the properties of the minimal model. In particular, the notion of "growth threshold" is fundamental. In a first section we establish the mathematical properties that we interpret in the following section and finally we produce some simulation. In a last section we propose four possible extensions of the minimal model. The mathematical treatment will be faster either because it does not present any difficulty for the reader who has assimilated the above or, on the contrary, because it is more delicate and falls outside the scope of this work.

Keywords: anaerobic digestion; steady state; mortality; stability; hyperbolic equilibria.

2010 AMS Subject Classification: 92C37.

1. INTRODUCTION

A bioreactor is an enclosure containing a nutrient medium composed of a cocktail of various, we speak of "substrates" on which grow one or more populations of microorganisms, all of these microorganisms, the whole being also called "biomass". Bioreactors are used to carry

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out operations for the transformation of matter by biological means which are most often, but not systematically, accompanied by an increase in the biomass in the reaction medium see [6]. Microbiology teaches us that only soluble substrates that have created chemical bonds with water molecules are available for the growth of living cells. In the context of this article, from a formal point of view, a biological reaction will therefore describe the passage of elements found in the medium in soluble form to a solid form, biomass and possibly in a certain number of metabolites and / or gas. However, there may be times when some resources are in solid form. A so called "hydrolysis" step is then necessary to transform this solid substrate into a soluble form which can be assimilated by microorganisms. The sight in which a microorganism "catches" molecules passing by it is like a sight of the mind. For example, it is believed in soils that most microorganisms, whether mobile or not, excrete enzymes around them and pick up nutrients that reach them by diffusion. It is therefore essential to distinguish between the different processes involved before embarking on the modeling of phenomena as complex as the degradation of a set of substrates by microorganisms. It is the object of this work to describe the most important processes involved in this type of transformation of systematic matter commonly adopted in process engineering to model them. In what follows, we will restrict ourselves to microbial ecosystems which are those used in most bioprocesses.

Anaerobic digestion is the degradation of organic matter in the absence of oxygen. The final product being methane, a renewable energy. This process is more and more used for the treatment of liquid and solid waste. Because of its relative instability due to the possible accumulation of intermediate products, notably the volatile fatty acids (VFA), the modeling of this process has been extensively studied over these last years. Such models are multi-step mass balance models in which the reactional network consists in a number of biological reactions taking place the medium in parallel and / or in series. Their complexity highly depends on the objectives by the modeler. On the one hand, when the objective is to develop models for integrating and formalize the available knowledge typically to better understand bioprocesses, models are generally high order models and not tractable from a mathematical viewpoint, cf. for instance the ADM1 [1]. On the other hand, when the aim of the modeling is to develop decision tools or control systems, low order models are better suited, as for instance the AM2 [3]. In this

second class of models, several two-steps models have been proposed in the literature.
Two steps models are commonly used to describe commensalistic microbial systems which take the form of a cascade of two biological reactions where one substrate S_1 is consumed by one microorganism/ecosystem X_1 to produce S_2 which serves as the main limiting substrate for a second microorganism/ecosystem X_2 as schematically represented by the following reaction scheme representing a simplified scheme of the anaerobic digestion

$$S_1 \xrightarrow{\mu_1(.)} X_1 + S_2, \quad S_2 \xrightarrow{\mu_2(.)} X_2 + CO_2 + CH_4.$$

The most general one-step model under interest in the actual paper can be written as:

$$\left\{ \begin{array}{l} \dot{S} = D(S^{in} - S) - \mu(.)\frac{X}{Y(.)}, \\ \\ \dot{X} = [\mu(.) - D]X, \end{array} \right. \tag{1}$$

where D is the dilution rate, while S^{in} is the input substrate concentration. Parameters $Y(.)$ is the yield coefficients associated to the bioreactions. The kinetics $\mu(.)$ is of Monod type.

The different analyses of the class of models (1) available in the literature essentially differ on the way the growth rate functions are characterized.

2. Mathematical Model

2.1. Mathematical properties of the minimal model. Throughout this section y (.) = Y is a constant. Function $S \Rightarrow \mu(S)$ is continuous and has a continuous derivative, is positive and null at 0. First we suppose that it is increasing then we introduce the possibility of inhibition phenomena by assuming it increasing then decreasing.

The one-step model reads:

$$\left\{ \begin{array}{l} \dot{S} = D(S^{in} - S) - \mu(S)X, \\ \\ \dot{X} = [\mu(S) - D]X, \end{array} \right. \tag{2}$$

where S is the substrate concentration introduced in the chemostat with input concentrations S^{in}. Where D is the dilution rate, X is the hydrolytic bacteria concentration. The functions $\mu : (S) \to \mu(S)$ is the specific growth rate of the bacteria. We call (2) the minimal model. The

existence and uniqueness theorem apply. Since it is assumed that μ has a continuous derivative, the second member of (2) has continuous partial derivatives and therefore the existence and uniqueness of solutions theorem applies.

We assume:

A1. The horizontal axis is invariant. indeed, we immediately check that for all $s(0)$ the function:

$$t \to (s(t),x(t)) = (s^{in} + (s(0) - s^{in})e^{-D}t, 0)$$

is a solution of (2).

A2. The solutions remain positive. As s and x are positive or zero quantities (concentrations), it is necessary to ensure that solutions with positive or zero initial conditions remain so. To do this, it suffices to note that:

$$s = 0 \Rightarrow \frac{ds}{dt} = Ds^{in} > 0$$

and therefore no trajectory can leave the positive orthan $\mathbb{R}^{+2}$ by crossing the vertical semi-axis. As the horizontal semi-axis is a trajectory and two trajectories cannot cross at any $\mathbb{R}^{+2}$ by crossing a horizontal semi-axis.

3. Analysis of the Model

3.1. The dynamics of s and x.

An invariant set. Let z = s + x. Derive:

$$\frac{dz}{dt} = \frac{ds}{dt} + \frac{dx}{dt} = D(s^{in} - s) - \mu(s)x + \mu(s)x(t) - Dx$$

$$\frac{dz}{dt} = D(s^{in} - s) - Dx = D(s^{in} - (s+x)) = D(s^{in} - z).$$

We can explicitly integrate:

$$\begin{cases} \frac{dz}{dt} = D(S^{in} - z), \\ \\ z(0) = s(0) + x(0), \end{cases} \tag{3}$$

then:

$$z(t) = s^{in} + ((s(0) + x(0)) - s^{in})e^{-Dt}.$$

We see that after a transient, we have:

$$s(t)+x(t) \approx s^{in}.$$

If the initial condition is such that $s(0)+x(0) = s^{in}$ we have exactly:

$$s(t)+x(t) = s^{in}.$$

The segment:

$$I = \{(s,x) : s \geq 0, x \geq 0, s+x = s^{in}\}$$

is therefore an attractive invariant set. On this set, since $s+x = s^{in}$ we can replace s by $s-x$ in the second equation of (1) which gives the differential equation in x

$$\frac{dx}{dt} = (\mu(s^{in}-s)-D)x.$$

Therefore the simple behavior is known as soon as we know the function graph $x :\to \phi(x) = (\mu(s^{in}-s)-D)x$. legality $s^{in} = s+x$ reflects the fact that in this model where the yield is equal to 1 the quantity of substrate consumed is transformed into an equal quality of biomass

- The solutions are bounded. This follows immediately from the fact that $t \to z(t)$ is a bounded function, that s + x = z, and that s and x are positive or zero.
- The balances. The equilibria of (1) are the solutions of:

$$\begin{cases} 0 = D(S^{in}-s)-\mu(s)x, \\ \\ 0 = (\mu(s)-D)x. \end{cases} \tag{4}$$

There is always a solution $(s^{in},0)$ called leaching solution. The other solutions are: (s^*,x^*), where s^* is a value of s such that $\mu(s^*) = D$ and $x^* = s^{in}-s^*$.

Remark 3.1. *the function μ is monotonic and bounded*

We assume that the function μ is of type Monod, that is:

- *μ is defined for $s \geq 0$ and bounded;*
- *Zero for $s = 0$;*
- *Such that $\mu'(s) > 0$ therefore strictly increasing.*

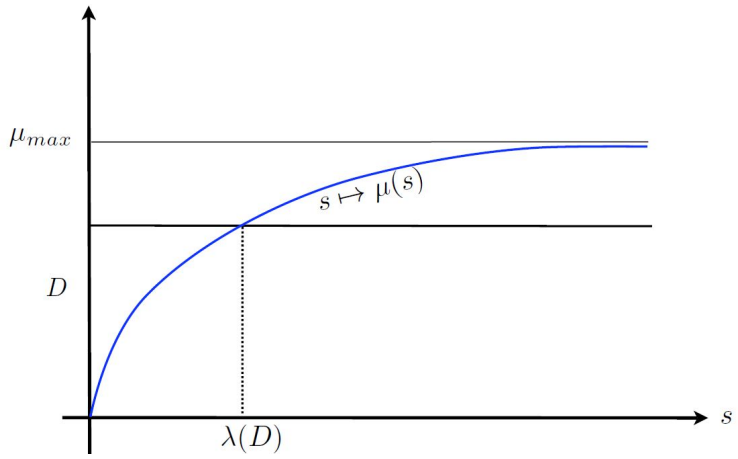

FIGURE 1. Monod-type function: existence and uniqueness of the solution of $\mu(s^*) = D$, we noted μ_{max} the upper limit not reached of μ

An increasing and bounded function has an upper bound which we note:

$$\mu_{max} = sup\mu(s).$$

The expression μ_{max} means maximum of μ, which is a little bit improper from a mathematical point of view since the upper limit of a strictly increasing function is never reached. The Monod fonction is the fonction:

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

It is obvious of Monod type and its upper bound is the parameter μ_{max}. The constant k_s is called the semi-saturation constant.

3.2. The Steady states. The steady states are the couples (s_e, x_e) for which the second members of (2) are zero, so $t :\to (s_e, x_e)$ is a constant solution of (2), therefore an equilibria.

(1) The first steady state is the Washout: $E_0 = (S_{in}, 0)$

(2) The steady state with biomass, When $D < \mu_{max}$ we denote the λ unique s such that $\mu(s) = D$ it is unique as $s \to \mu(s)$ is strictly increasing, otherwise, we note $\lambda(D) = +\infty$. If $s < \lambda(D)$ the growth rate of x:

$$\frac{dx}{dt} = (\mu(s) - D)x$$

is strictly minus, whereas if $s > \lambda(D)$ the growth rate is strictly positive.

Remark 3.2. *The quantity $\lambda(D)$ is called the growth threshold.*

Either $D < \mu(S_{in})$; let's set $s^* = \lambda(D)$ et $x^* = S_{in} - s^*$ so :

$$E_1 = (s^*, x^*)$$

Steady state with positive biomass, fact, on the one hand $s^* = \lambda(D) \Rightarrow \frac{dx}{dt} = (\mu(s^*) - D)x^* = 0$, and on the other hand by adding the two second members we obtain:

$$0 = D(S_{in} - s^* - x^*)$$

hence: $x^* = S_{in} - s^*$.

If $D > \mu(S_{in})$ we have $s^* = \lambda(D) > S_{in}$ and the equation $0 = D(S_{in} - s^* - x)$ has no solution with $x > 0$ (see following figures)

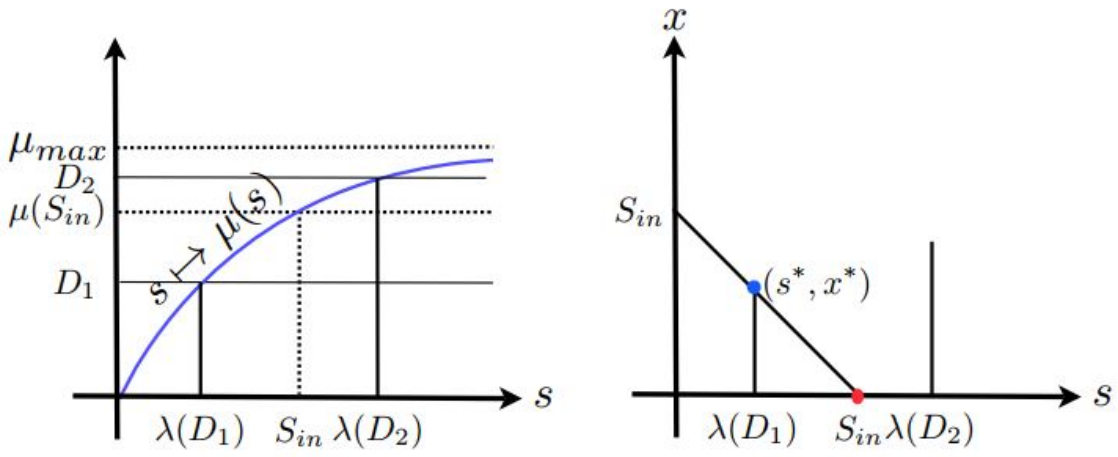

FIGURE 2. Steady state: Washout equilibrium (red), the steady state with positive biomass (blue) exists only for $D < \mu(S_{in})$

4. LOCAL STABILITY OF EQUILIBRIA

We know that an equilibrium is locally exponentially stable if the real parts of the eigenvalues of the Jacobian matrix at this point are strictly negative. See [4]. The Jacobian matrix in (s,x)

of (2)

$$J(s,x) = \begin{bmatrix} -D-\mu' x & -\mu(s) \\ \\ \mu' x & \mu(s)-D \end{bmatrix}. \tag{5}$$

The Washout equilibrium evaluated in $E_0 = (S_{in}, 0)$ the jacobian matrix is:

$$J(E_0) = \begin{bmatrix} -D & -\mu(S_{in}) \\ \\ 0 & \mu(S_{in})-D \end{bmatrix}. \tag{6}$$

The two eigenvalues are $-D$ and $\mu(S_{in}-D)$. So if $D > \mu(S_{in})$ it is a locally exponentially stable steady state (LES), if $D < \mu(S_{in})$ it is an unstable steady state.

The steady state with biomass. For $D < \mu(S_{in})$, the jacobian matrix at $E_1 = (s^*, x^*)$ is:

$$J(E_1) = \begin{bmatrix} -D-\mu'(s^*)(x^*) & -\mu(s^*) \\ \\ \mu'(s^*)(x^*) & (\mu(s^*)-D)x^* \end{bmatrix}. \tag{7}$$

But, since $s^* = \lambda(D)$, we have $\mu(s^*) = D$ and the jacobian matrix reduces to:

$$J(E_1) = \begin{bmatrix} -D-\mu'(s^*)(x^*) & -D \\ \\ \mu'(s^*)(x^*) & 0 \end{bmatrix}. \tag{8}$$

The trace is strictly negative, and the determinant positive, so the eigenvalues have strictly negative real parts. This equilibrium is therefore locally exponentially stable and as the roots are real there is no oscillation around the equilibrium. The expression locally means that if the initial conditions are close enough to the equilibrium the solutions tend towards the equilibrium; This information is summarized in the table (1).

S_{in}	$\lambda(D) < S_{in}$	$\lambda(D) = S_{in}$	$\lambda(D) > S_{in}$
E_0	unstable	Stable	LES
E_1	LES	does not exist	does not exist

TABLE 1. Local stability of the steady state of (2) for μ Monod-type

5. The Operating Diagram

Apart from the two operating (or control) parameters, which are the input substrate concentration D_{in} and the dilution rate D that can vary, all others parameters have biological meaning and are fixed depending on the organisms and substrate considered. The operating diagram shows how the system behaves when we vary the two control parameters S_{in} and D. See [5]

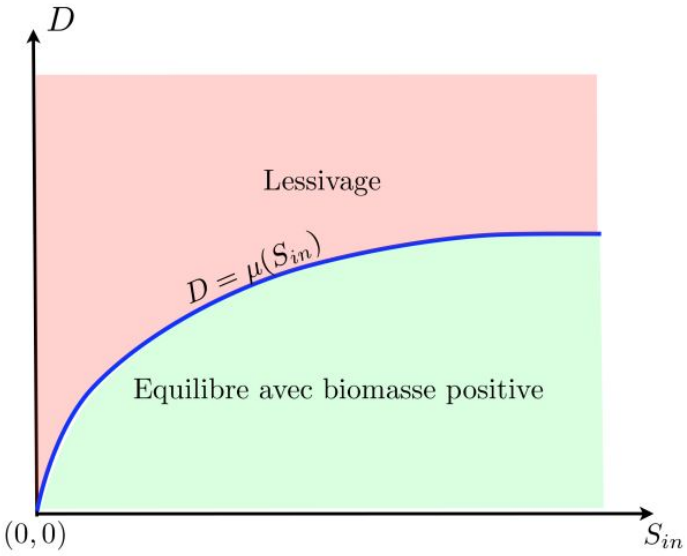

FIGURE 3. The operating diagram for the system (2): the stability regions of each Steady state, E_1 and E_2

6. Conclusions

In this paper, we have presented an analysis of an anaerobic digestion model in which we considered two stages corresponding to hydrolysis and methanogenesis phases. We have considered a non usual growth function for hydrolysis step that is the Monod growth function which gave us two steady state E1 and E2 and each has its condition of existence and stability. In the next work we will study the methanogenesis stage using the Haldane and Contois growth function to make the comparison.

Conflict of Interests

The authors declare that there is no conflict of interests.

REFERENCES

[1] D.J. Batstone, J. Keller, I. Angelidaki, et al. The IWA anaerobic digestion model No 1 (ADM1), Water Sci. Technol. 45 (2002), 65–73. https://doi.org/10.2166/wst.2002.0292.

[2] T. Sari, J. Harmand, A model of a syntrophic relationship between two microbial species in a chemostat including maintenance, Math. Biosci. 275 (2016), 1–9. https://doi.org/10.1016/j.mbs.2016.02.008.

[3] I. Ramirez, A. Mottet, H. Carrère, et al. Modified ADM1 disintegration/hydrolysis structures for modeling batch thermophilic anaerobic digestion of thermally pretreated waste activated sludge, Water Res. 43 (2009), 3479–3492. https://doi.org/10.1016/j.watres.2009.05.023.

[4] J. Harmand, C. Lobry, A. Rapaport, et al. The chemostat: Mathematical theory of microorganism cultures, Wiley, London, 2017.

[5] Z. Khedim, B. Benyahia, B. Cherki, et al. Effect of control parameters on biogas production during the anaerobic digestion of protein-rich substrates, Appl. Math. Model. 61 (2018), 351–376. https://doi.org/10.1016/j.apm.2018.04.020.

[6] G. Stephanopoulos, The dynamics of commensalism, Biotechnol. Bioeng. 23 (1981), 2243–2255. https://doi.org/10.1002/bit.260231008.

[7] P.J. Reilly, Stability of commensalistic systems, Biotechnol. Bioeng. 16 (1974), 1373–1392. https://doi.org/10.1002/bit.260161006.

[8] M. Sbarciog, M. Loccufier, E. Noldus, Determination of appropriate operating strategies for anaerobic digestion systems, Biochem. Eng. J. 51 (2010), 180–188. https://doi.org/10.1016/j.bej.2010.06.016.

[9] B. Benyahia, T. Sari, B. Cherki, J. Harmand, Bifurcation and stability analysis of a two step model for monitoring anaerobic digestion processes, J. Process Control. 22 (2012), 1008–1019. https://doi.org/10.1016/j.jprocont.2012.04.012.

[10] O. Bernard, Z. Hadj-Sadok, D. Dochain, et al. Dynamical model development and parameter identification for an anaerobic wastewater treatment process, Biotechnol. Bioeng. 75 (2001), 424–438. https://doi.org/10.1002/bit.10036.