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To cite this version:

Boumediene Benyahia, Tewfik Sari, Brahim Cherki, Jérôme Harmand. Anaerobic Membrane BioReactor modeling in the presence of Soluble Microbial Products (SMP) - the Anaerobic Model AM2b. Chemical Engineering Journal, 2013, 228, pp.1011-1022. 10.1016/j.cej.2013.05.073 . hal-00859541

HAL Id: hal-00859541

https://inria.hal.science/hal-00859541v1

Submitted on 16 May 2020

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The original publication is available at http://www.sciencedirect.com.
DOI : 10.1016/j.cej.2013.05.073

Anaerobic Membrane BioReactor modeling in the presence of Soluble Microbial Products (SMP) - the Anaerobic Model AM2b

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Abstract

In this paper, we develop a mathematical model of anaerobic membrane bioreactors (AnMBR) for control design purposes. In particular, we integrate into this model the production and the degradation of Soluble Microbial Products (SMP), which are known to play an important role in the membrane fouling phenomenon. The proposed model, named AM2b, is based on the modification of the AM2 two step model initially proposed in [1]. We present a graph-based approach to determinate its equilibria and discuss three different generic cases. We show that under general assumptions (case A), the model developed has the same number of equilibria as the AM2 model and operates in bi-stability [2]. However, under certain operating conditions or if

☆This work was supported by *AiresSud* (project 7015), *Coadvise* (project FP7-PEOPLE-IRSES-2008 No. 230833) and *Treasure* (an Inria Euromed 3+3 project, http://project.inria.fr/treasure/). This article is an extension of the IFAC 2011 proceeding [3].

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DOI : 10.1016/j.cej.2013.05.073

biological parameters values are slightly modified (cases B and C), the AM2b model exhibits equilibria bifurcation and multi-stability property. It is also shown that the AM2b model can provide interesting qualitative information to the user, such as the influence on some equilibria of the variation in the concentration of organic matter in the influent concentration.
Keywords: Anaerobic digestion; Equilibria bifurcation; Membrane fouling; MBR; SMP Modeling; Wastewater treatment plant.

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1. Introduction

The objectives of a wastewater treatment plant (WWTP) are to reduce the volume of pollutants in discharges, take advantage of the energy that can potentially be produced (such as CH_4 in anaerobic treatment) and provide purified effluents for recycling in agriculture and/or industry. The technology of Anaerobic Membrane BioReactors (AnMBR) appears promising for achieving these aims. However, the risk of membrane fouling limits the development of these systems. The use of models coupling the fouling phenomena together with biotic characteristics should enable such fouling to be more predictable and thus, by means of a control, to act in order to limit their impact on system performance.

Among the soluble organic compounds in WWTP effluent, it has been shown that the Soluble Microbial Products (SMP) play a crucial role in the membrane fouling (pore blocking) and their presence in a MBR affects the process performance (effluent quality). It is therefore essential to integrate the SMP into the modeling of bioprocesses.

Most efforts to couple biotic phenomena with membrane models have been

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primarily directed at improving aerobic systems. They have been based on the modification of activated sludge models (ASM) to include SMP formation and degradation. Concerning anaerobic conditions, in contrast, only a few papers are available [4]. Yet anaerobic digestion systems offer many advantages, including the possible use of the resulting biogas as an energy source. Usually, two categories of SMP are considered: BAP (Biomass Associated Products), associated with biomass mortality, and UAP (Utilization Associated Products), associated with substrate degradation and the growth of biomass [5].

In their review [5], Barker and Stuckey noted that the first model to characterize *only* the SMP formation in a fermentation system was proposed in 1959 by Luedeking and Piret [6]. Later on, this incomplete model was further refined. But the first model to predict *both* the production and the degradation of SMP in an anaerobic chemostat was proposed by [7], in considering the two categories of SMP (UAP and BAP). It integrated the UAP production but starting from the initial organic matter alone and considered only their degradation by acidogenic bacteria. The BAP were considered to be produced by the decay of acidogenic bacteria and also slowly degraded by them. The model did not take into account either the UAP or BAP production starting from the intermediate product of the reaction (a two step model was considered), nor the decay of methanogenic biomass.

This model was further developed by [8] who have added: i) the concept of UAP production in the consumption of both the initial organic matter and the intermediate products by acidogenic and methanogenic bacteria respectively; ii) BAP production starting from the decay of acidogenic and

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methanogenic bacteria; and iii) BAP degradation by acidogens which grow and give intermediate products.

Later on, [9] proposed a unified theory for the production and the degradation of the UAP and the BAP by envisaging the combination of three types of compound: Extracellular Polymeric Substances (EPS), SMP and inert biomass. They organized their theory through six hypothetical interactions between SMP, EPS, active and inert biomass.

Recently, Aquino and Stuckey [10] in order to predict SMP production, have refined the model suggested in [8] by taking into account the concept of EPS formation and degradation as suggested in [9].

It should be stressed that the majority of the studies cited above relate to conventional systems for anaerobic digestion (chemostat-like systems) and not to membrane reactors. In addition, the most recently developed models are rather complex and clearly unsuited for observer synthesis and/or control system design.

This paper proposes a model which includes the formation and degradation of SMP in an AnMBR, and should prove simple enough to be used for control purposes while capturing the main features related to SMP dynamics. To this end, we propose the AM2b model which we study equilibria and their bifurcations.

This paper is structured as follows: first, we present the model with SMP. Its equilibria are then determined for different generic cases using a graph-based approach. Finally, simulation results are presented which point out different qualitative behavior according to model parameters values. These simulations are discussed before conclusions and perspectives are drawn.

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2. Development of AM2b model

2.1. Hypotheses

The compartments included in the model are represented in Fig. 1. The process considered here is a side-stream MBR, where S_1 is the organic matter concentration (COD), S_{1in} the input concentration, S_2 the Volatile Fatty Acid concentration (VFA), S_{2in} the input concentration, X_1 the acidogenic biomass, X_2 the methanogenic biomass and $S = UAP + BAP$ *i.e.* the Soluble Microbial Products (SMP) concentration.

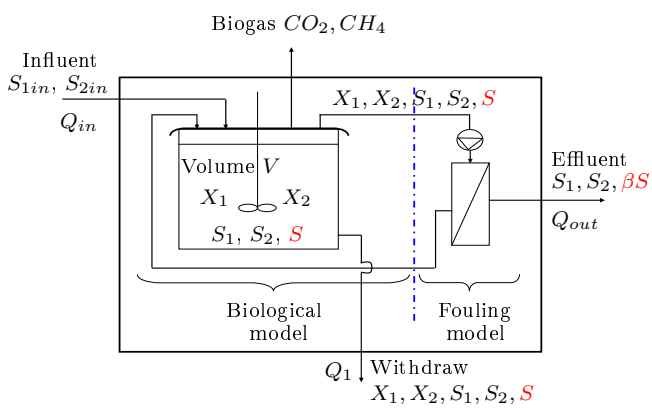

Figure 1: Schematic representation of the proposed model.

A full model of an AnMBR should integrate a biological model of bioreactions taking place in the reaction medium along with a membrane fouling model. In this paper, we develop only the biological model under the following assumptions:

H1. The reaction medium of the bioreactor is considered to be homogeneous,

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H2. The substrates S_1 and S_2 go through the external membrane without retention (the size of their molecules is assumed to be smaller than pore diameter),

H3. Total retention of biomasses X_1 and X_2 by the membrane is considered (the size of bacteria is greater than pore diameter). Therefore, there are no solids in the effluent and thus no term $-DX_i$ in the mass balance equation of X_i (see equations (8) and (10)),

H4. Decay rates of biomasses noted D_0 are taken into account,

H5. The biomass withdrawal with a flowrate Q_1 is considered,

H6. $SMP = UAP + BAP$ are grouped into a single variable of concentration S, of which only a fraction β leaves the bioreactor. The remainder, corresponding to macromolecules, is retained by the membrane. This is modeled in the mass balance equation by $-\beta DS$ (see equation (11)), where $0 \leq \beta \leq 1$ ($\beta = 0$ stands for the total retention of SMP by the membrane while $\beta = 1$ means free crossing of SMP through the membrane).

On the left of Fig. 2 is represented the separation of matter by the membrane which is formalized through assumptions H2, H3 and H6. On the right is shown the linear working zone of the bioreactor, when the membrane flow J evolves proportionally to the transmembrane pressure ΔP.

2.2. Reaction network and mathematical model

Our model is based on the modification of the two-step model AM2 proposed in [1] that has been analyzed by [11] in a chemostat and by [2] in a

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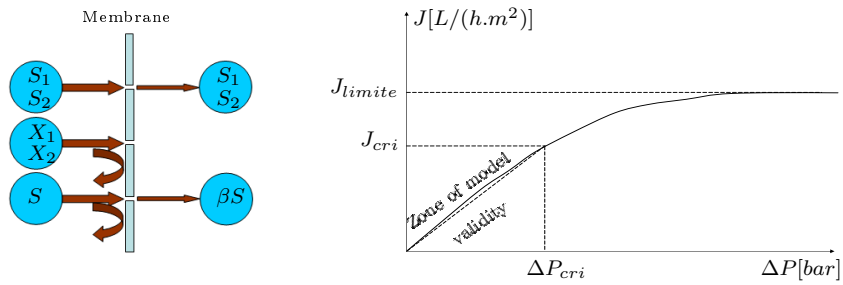

Figure 2: Left: Separation of matter by the membrane. Right: Flux variation depending on transmembrane pressure.

more generic case. In such models, anaerobic digestion is considered as a two-step process:

- first, acidogenesis in which a consortium of acidogenic bacteria X_1 consume the organic substrate S_1 and produce CO_2 and S_2 (VFA):

$$k_1 S_1 \xrightarrow{r_1} X_1 + k_2 S_2 + k_4 CO_2. \tag{1}$$

- second, methanogenesis where a consortium of methanogenic bacteria X_2 use S_2 as substrate to grow and then produce biogas composed of CO_2 and CH_4:

$$k_3 S_2 \xrightarrow{r_2} X_2 + k_5 CO_2 + k_6 CH_4. \tag{2}$$

We proved in [2] that the AM2 model has at most six equilibrium points and that it can exhibit a bistability. Here, we propose to modify the reaction network (1)-(2) by adding a new compound SMP, named S. We model the SMP production from the degradation of S_1, S_2 and the decay of biomasses

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X_1, X_2. In addition, we consider the SMP degradation into S_2 and CO_2 through the growth of X_1. The corresponding reaction networks are given as follows:

- Acidogenesis + SMP production:

$$k_1 S_1 \xrightarrow{r_1} X_1 + k_2 S_2 + b_3 S + k_4 CO_2, \tag{3}$$

  with the reaction rate: $r_1 = \mu_1(S_1)X_1$.

- Methanogenesis + SMP production:

$$k_3 S_2 \xrightarrow{r_2} X_2 + b_4 S + k_5 CO_2 + k_6 CH_4, \tag{4}$$

  with the reaction rate: $r_2 = \mu_2(S_2)X_2$.

- SMP degradation:

$$b_1 S \xrightarrow{r} X_1 + b_2 S_2 + k_7 CO_2, \tag{5}$$

  with the reaction rate: $r = \mu(S)X_1$.

- SMP production from biomass decay:

$$D_0 X_1 \longrightarrow D_0 S, \qquad D_0 X_2 \longrightarrow D_0 S. \tag{6}$$

Let us note $\xi = [S_1, X_1, S_2, X_2, S]^T$ the state space vector of the model AM2+SMP (henceforth, this model is named "AM2b"). From the reaction network (3)-(6) and taking into account the above assumptions (H1-H6), the

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law of the conservation of matter enables us to write the following mathematical model:

$$\frac{dS_1}{dt} = D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1, \tag{7}$$

$$\frac{dX_1}{dt} = \Big(\mu_1(S_1) + \mu(S) - D_0 - D_1\Big)X_1, \tag{8}$$

$$\frac{dS_2}{dt} = D(S_{2in} - S_2) - k_3\mu_2(S_2)X_2 + \Big(k_2\mu_1(S_1) + b_2\mu(S)\Big)X_1, \tag{9}$$

$$\frac{dX_1}{dt} = \Big(\mu_2(S_2) - D_0 - D_1\Big)X_2, \tag{10}$$

$$\frac{dS}{dt} = \Big(b_3\mu_1(S_1) + D_0 - b_1\mu(S)\Big)X_1 + \Big(b_4\mu_2(S_2) + D_0\Big)X_2 - MS, \tag{11}$$

with:

k_1: degradation rate of S_1 by X_1,

k_2: production rate of S_2 by X_1 from S_1,

k_3: degradation rate of S_2 by X_2,

b_1: degradation rate of S by X_1,

b_2: production rate of S_2 by X_1 from S,

b_3: production rate of S by X_1 from S_1,

b_4: production rate of S by X_2 from S_2,

β: SMP fraction leaving the bioreactor,

D: dilution rate ($= Q_{in}/V$),

D_0: decay rate of biomass,

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D_1: withdrawal of biomass $(= Q_1/V\ )$,

$M = [\beta D + (1-\beta)D_1]$: constant.

Remark 1. : Substituting $S = 0$ in the equations (7)-(10) gives the four dimensional model AM2 [1].

Certain biological conditions must prevail in the reaction networks (3), (4) and (5):

- over a given period of time, the quantity of biomass (or products) produced is always smaller than the quantity of substrate consumed (see (4) and (5)). Thus, one has:

$$k_3 \geq 1 + b_4, \tag{12}$$

$$b_1 \geq 1 + b_2. \tag{13}$$

- the quantity S_2 of VFA produced from S_1 is higher than the quantity produced from the SMP (see (3) and (5)):

$$k_2 > b_2. \tag{14}$$

3. Equilibria of model

3.1. Characterization of equilibria

The kinetics μ_1, μ_2 and μ are assumed to be dependent on S_1, S_2 and S, respectively. The model analysis given in this paper is valid for all kinetics verifying the following qualitative properties whose patterns are represented as graphs in Fig. 3:

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1. $\mu_1(S_1)$ and $\mu(S)$ are increasing functions for $S_1 \geq 0$ and $S \geq 0$ respectively, with $\mu_1(0) = \mu(0) = 0$, and $\mu_1(+\infty) = m_1$ and $\mu(+\infty) = m$.
2. $\mu_2(S_2)$ is an increasing function for $0 \leq S_2 < S_2^M$; it has a maximum $\mu_2\left(S_2^M\right) > 0$ for $S_2 = S_2^M$ and it is decreasing for $S_2 > S_2^M$, with $\mu_2(0) = 0$ and $\mu_2(+\infty) = 0$.

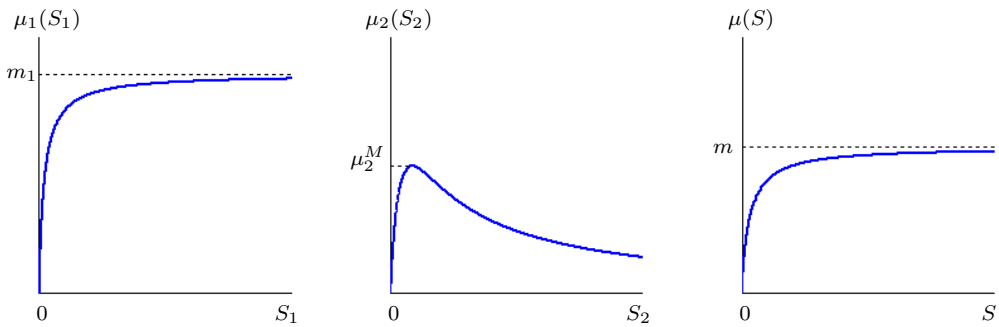

Figure 3: Schematic representation of the kinetic properties.

Examples of such kinetics (used in the sequel) are the Monod functions for μ_1 and μ and the Haldane function for μ_2.

$$\mu_1(S_1) = m_1 \frac{S_1}{S_1 + K_1}, \qquad \mu(S) = m \frac{S}{S + K}, \qquad \mu_2(S_2) = m_2 \frac{S_2}{\frac{S_2^2}{K_i} + S_2 + K_2}. \quad (15)$$

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The equilibria of system (7)-(11) are solutions of the following nonlinear algebraic system:

$$
\begin{aligned}
0 &= D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1, && (16)\\
0 &= \Big(\mu_1(S_1) + \mu(S) - D_0 - D_1\Big)X_1, && (17)\\
0 &= D(S_{2in} - S_2) - k_3\mu_2(S_2)X_2 + \Big(k_2\mu_1(S_1) + b_2\mu(S)\Big)X_1, && (18)\\
0 &= \Big(\mu_2(S_2) - D_0 - D_1\Big)X_2, && (19)\\
0 &= \Big(b_3\mu_1(S_1) + D_0 - b_1\mu(S)\Big)X_1 + \Big(b_4\mu_2(S_2) + D_0\Big)X_2 - MS, && (20)
\end{aligned}
$$

which is obtained from (7)-(11) by setting the right-hand sides at zero. Three cases are considered:

Case 1. Washout of X_1 :

The equilibria $(S_1^*, X_1^*, S_2^*, X_2^*, S^*)$ of the system (7)-(11) for which $X_1^* = 0$ are given by:

- the washout equilibrium of X_1 and X_2, $E_0^0 = (S_{1in}, 0, S_{2in}, 0, 0)$, which always exists,
- the washout equilibrium of X_1 but not of X_2, $E_1^i = (S_{1in}, 0, S_2^{i*}, X_2^{i*}, S^{i*})$, $i = 1$ or 2,

  X_2^{i*} and S^{i*} are given by the formulas:

$$X_2^{i*} = \frac{D(S_{2in} - S_2^{i*})}{k_3(D_0 + D_1)}, \quad S^{i*} = \frac{b_4 + \frac{D_0}{D_0+D_1}}{Bk_3}(S_{2in} - S_2^{i*}), \quad i = 1, 2,$$

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where S_2^{i*} are the roots of equation $\mu_2(S_2) = D_0 + D_1$ and,

$$B = \left[\beta + (1-\beta)\frac{D_1}{D}\right] = \frac{M}{D}.$$

The equilibrium E_1^i exists if and only if:

$$S_{2in} > S_2^{i*}. \tag{21}$$

Case 2. Washout of X_2 but not of X_1 :

Let $E^* = (S_1^*, X_1^*, S_2^*, X_2^*, S^*)$ an equilibrium point of system (7)-(11). If $X_1^* > 0$ and $X_2^* = 0$ then one has $0 < S_1^* < S_{1in}$, $S_2^* > 0$ and $S^* > 0$. Moreover S_1^* and S^* are solutions of the system of equations:

$$\begin{cases} S_1 = F_m(S), \\ S = G(S_1) \end{cases} \tag{22}$$

where F_m and G are defined by:

$$F_m(S) := \mu_1^{-1}\Big(D_0 + D_1 - \mu(S)\Big), \tag{23}$$

$$G(S_1) := (S_{1in} - S_1)\left(B_1 + \frac{B_2}{\mu_1(S_1)}\right), \tag{24}$$

with:

$$B_1 = \frac{b_3 + b_1}{k_1 B}, \quad B_2 = \frac{D_0 - b_1(D_0 + D_1)}{k_1 B}. \tag{25}$$

X_1^* and S_2^* are given by the formulas:

$$X_1^* = D\frac{S_{1in} - S_1^*}{k_1\mu_1(S_1^*)}, \qquad S_2^* = S_{2in} + \left[k_2\mu_1(S_1^*) + b_2\mu(S^*)\right]\frac{S_{1in} - S_1^*}{k_1\mu_1(S_1^*)}.$$

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The equilibrium E^* exists if and only if:

$$S_{1in} > S_1^*. \tag{26}$$

Case 3. No washout of X_1 and X_2 :

Let $E^* = (S_1^*, X_1^*, S_2^*, X_2^*, S^*)$ an equilibrium point of system (7)-(11). If $X_1^* > 0$ and $X_2^* > 0$, then one has $0 < S_1^* < S_{1in}$, $S_2^* = S_2^{i*}$, $i = 1, 2$ and $S^* > 0$. Moreover, S_1^* and S^* are solutions of the system of equations:

$$\begin{cases} S_1 = F_m(S), \\ S = H_i(S_1), \quad i{=}1, 2. \end{cases} \tag{27}$$

where H_i, $i = 1, 2$ are defined by:

$$H_i(S_1) \;:=\; C_{1i} + (S_{1in} - S_1)\left(C_2 + \frac{C_3}{\mu_1(S_1)}\right), \quad i = 1, 2, \tag{28}$$

with:

$$C_{1i} = \frac{A}{B}(S_{2in} - S_2^{i*}), \;\; C_2 = \frac{A(k_2 - b_2) + b_3 + b_1}{k_1 B}, \;\; C_3 = \frac{(Ab_2 - b_1)(D_0 + D_1) + D_0}{k_1 B}, \tag{29}$$

$$A = \frac{b_4(D_0 + D_1) + D_0}{k_3(D_0 + D_1)}. \tag{30}$$

X_1^* and X_2^* are given by the formulas:

$$X_1^* = D\frac{S_{1in} - S_1^*}{k_1\mu_1(S_1^*)}, \qquad X_2^{i*} = D\frac{\left[S_{1in} - S_1^*\right]\left[k_2\mu_1(S_1^*) + b_2\mu(S^*)\right] + (S_{2in} - S_2^{i*})k_1\mu_1(S_1^*)}{k_1 k_3(D_0 + D_1)\mu_1(S_1^*)}.$$

The equilibrium E^* exists if and only if the condition (26) holds to-

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gether the following condition:

$$H_i(S_1^*) > G(S_1^*), \quad i = 1, 2. \tag{31}$$

The solutions of the system (16)-(20) are summarized in Fig. 4:

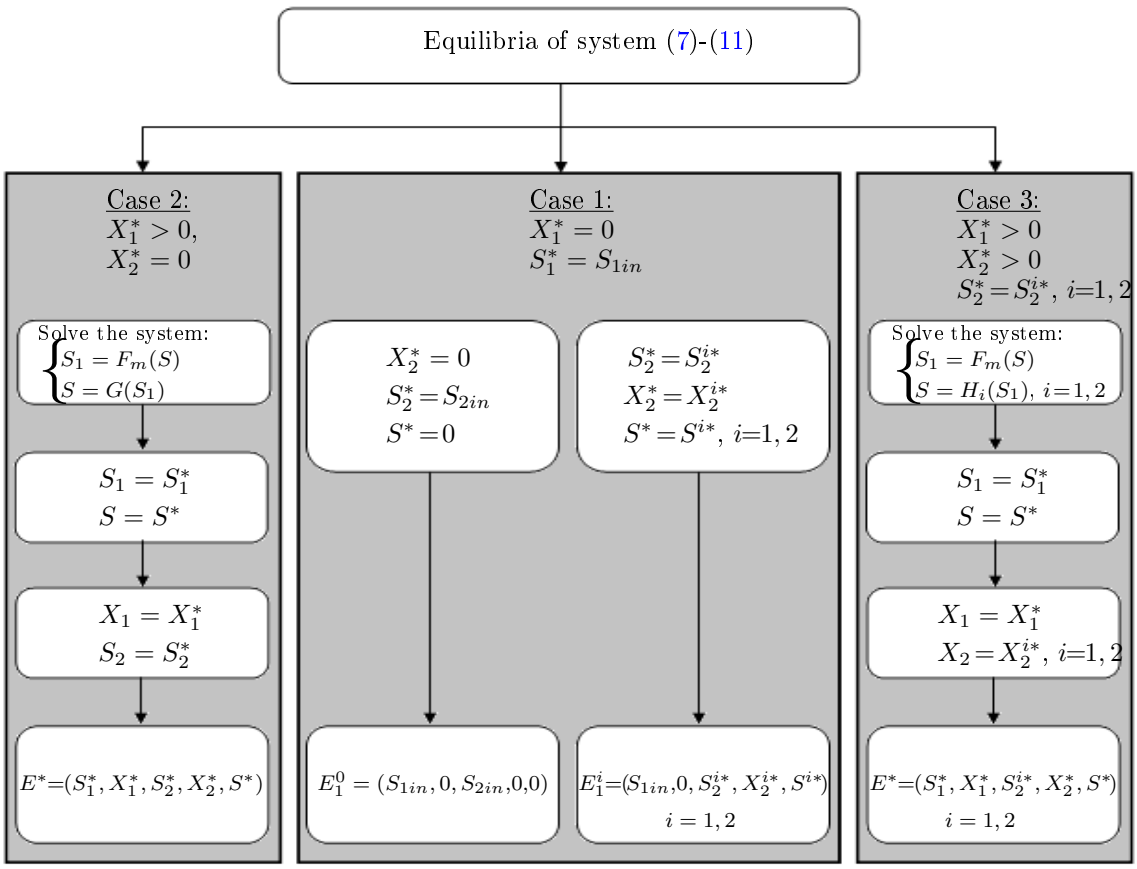

Figure 4: Diagram summarizing the equilibria of system (7)-(11).

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3.2. Graphical determination of equilibria

In this section, we propose a graph-based approach to determine the equilibria of system (7)-(11). It should be noted that only the positive values of S_1^* and S^*, which verify conditions (26) and (31) are considered.

Using (12) and (13), we show that $B_2 < 0$ and $C_3 < 0$. Hence G and H_i tend to $-\infty$ as S_1 tends to 0. We assume that $B_2 > -m_1 B_1$, $C_3 > -m_1 C_2$, so that G and H_i tend to $-\infty$ as S_1 tends to $+\infty$. Thus, the functions G and H_i are as in Figs. 5, 6 and 7. These figures are obtained with functions (15) and the values for biological parameters given in Table 1 (see below for cases A, B and C).

The parameters of the part of the model part without SMP (original model AM2) have values equal or close to the AMOCO values [1] (by using the standard deviation, see Table III in [1]). The other parameters b_1, b_2, b_3 and b_4 (the parameters of the part modeling the SMP), have values satisfying conditions (12), (13) and (14) and are chosen according to:

- $b_1 < k_1$: S is slowly degraded in relation to S_1,
- $b_3 < k_2$: the quantity of S_1 transformed in S_2 is higher than the quantity transformed in S,
- $b_4 < k_1, k_2, k_3$: the quantity of S_2 transformed in S is smaller than other quantities produced or degraded.

Units of yield coefficients are in $[g/g]$; concentrations, inhibition and half-saturation constants are in $[g/l]$; dilution rates, decay rates and maximum growth rates are in $[1/d]$.

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Table 1: Nominal values for the parameters of the AM2b model

Parameter	Value	Parameter	Value	Parameter	Value
m_1	1.2	β	0.6	b_2	0.6
K_1	10, 16 or 18	k_1	25	b_3	7
m_2	1.5	k_2	15	b_4	5
K_2	0.3	k_3	16.08	m	varying
K_I	0.9	b_1	5	K	3
D	1	D_0	0.25	D_1	0.4 or 0.25
S_{1in}	15 or 10	S_{2in}	1 or 0.6		

The difference between Figs. 5, 6 and 7 consists in the values of the parameters K_1, S_{1in}, S_{2in} and D_1. More precisely, we have:

- **Generic Case A**: $K_1 = 10$, $S_{1in} = 15$, $S_{2in} = 1$ and $D_1 = 0.4$ (see Fig. 5),
- **Generic Case B**: $K_1 = 16$, $S_{1in} = 15$, $S_{2in} = 1$ and $D_1 = 0.4$ (see Fig. 6),
- **Generic Case C**: $K_1 = 18$, $S_{1in} = 10$, $S_{2in} = 0.6$ and $D_1 = 0.25$, (see Fig. 7),

with $\lambda_1 = \mu_1^{-1}(D_0 + D_1)$.

In all cases, we vary the value of the bifurcation parameter m to change the form of $F_m(S)$ since it depends on this parameter of $\mu(S)$ (see (23)). Since functions $H_i(S_1)$ and $G(S_1)$ do not depend on the kinetics $\mu(S)$, their graphs do not change with m (see (24), (28) and Figs. 5, 6 and 7).

Notice that $F_m(S)$ can have zero, one or two intersections with $H_1(S_1)$, $H_2(S_1)$ or $G(S_1)$ (see Figs. 5, 6, and 7). Let us use the following notations for equilibria:

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- E^1_{2j}: equilibria given by the intersection of $F_m(S)$ with $H_1(S_1)$, $j = 1, 2$,
- E^2_{2j}: equilibria given by the intersection of $F_m(S)$ with $H_2(S_1)$, $j = 1, 2$,
- E^0_{2j}: equilibria given by the intersection of $F_m(S)$ with $G(S_1)$, $j = 1, 2$.

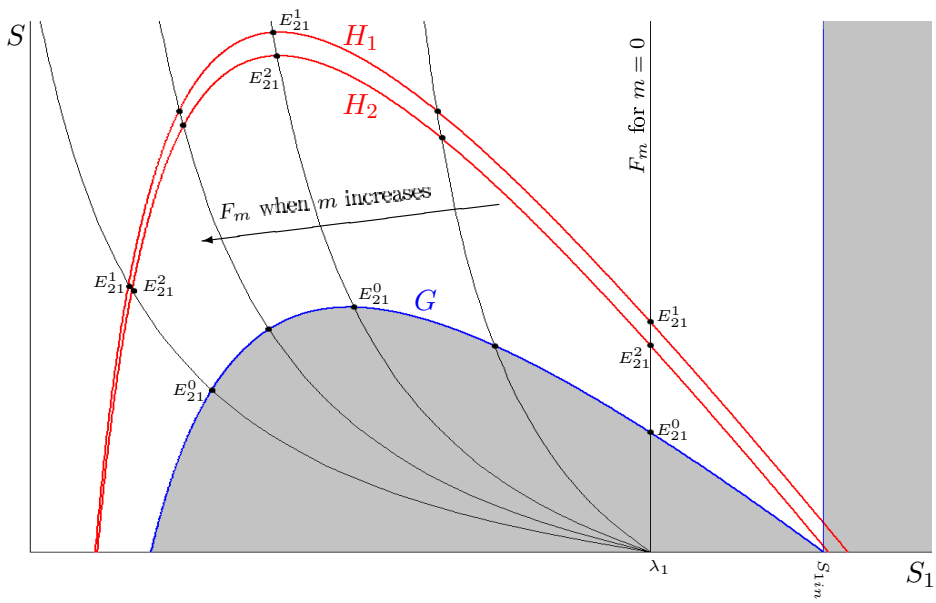

Figure 5: Intersection of the graph of $F_m(S)$ with the graphs $G(S_1)$ and $H_i(S_1)$ in the Case A.

Areas where the condition (26) and/or the condition (31) are not satisfied have been colored in gray. Therefore, any intersection of $F_m(S)$ with $H_1(S_1)$ or $H_2(S_1)$ which is within these areas is not considered.

4. Numerical simulations

In this section, we analyze the three generic cases illustrated by Figs. 5, 6 and 7. We characterize the number and the nature of equilibria according to the bifurcation parameter m. In addition, we highlight the capability of

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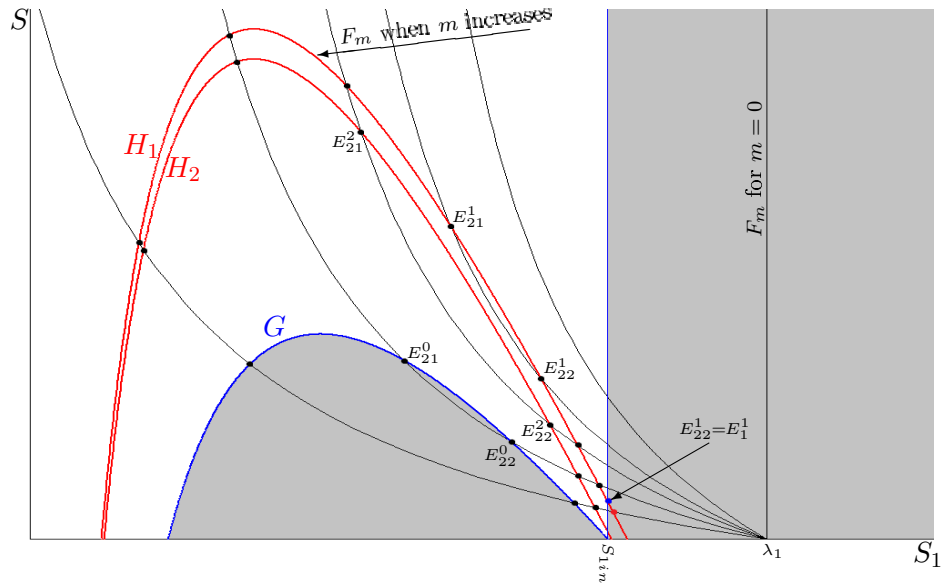

Figure 6: Intersection of the graph of $F_m(S)$ with the graphs $G(S_1)$ and $H_i(S_1)$ in the Case B.

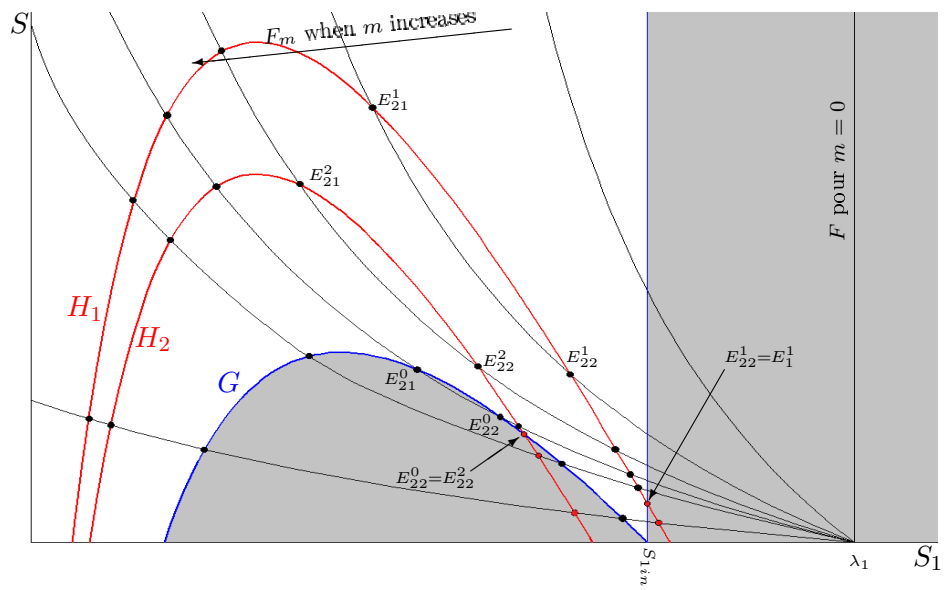

Figure 7: Intersection of the graph of $F_m(S)$ with the graphs $G(S_1)$ and $H_i(S_1)$ in the Case C.

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the AM2b model to predict a number of qualitative features of interest from a practical point of view.

4.1. Generic Case A: No equilibria bifurcation of AM2b

Case A is illustrated in Fig. 5. The intersection of the graph of $F_m(S)$ with graphs of $G(S_1)$, $H_1(S_1)$ and $H_2(S_1)$ give three equilibria E_{21}^0, E_{21}^1 and E_{21}^2 whatever the value of m (in addition to the trivial equilibria). The system keeps the number and the nature of its equilibria. Only the values of their components change when m varies, as represented in Fig. 9. The trivial equilibria E_0^0, E_1^1 and E_1^2 are represented in Fig. 8: they exist if and only if (21) holds and they do not depend on the parameter m. Here, we have:

$$S_2^{1*} = 0.3123 < S_2^{2*} = 0.8647 < S_{2in} = 1 \tag{32}$$

In total, the system can have six equilibria, summarized in Table 2, where T stands for *Trivial Equilibria*, while $F_m \cap H_1$, $F_m \cap H_2$ and $F_m \cap G$ stand for *Equilibria obtained by the intersections of the graph* F_m *with graphs* H_1, H_2 *and* G, respectively, and where S and U stand for a *Stable* and an *Unstable* Equilibrium, respectively.

Table 2: Equilibria and their nature in the generic case A represented in Fig. 5.

case A	Equilibria and nature					
	T			$F_m \cap G$	$F_m \cap H_2$	$F_m \cap H_1$
	E_0^0	E_1^1	E_1^2	E_{21}^0	E_{21}^2	E_{21}^1
$m \geq 0$	U	U	U	S	U	S

According to these results, we conclude that in operating conditions of the generic case A, the original system AM2, modified by the introduction

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of the new variable S, keeps the number and the nature of its equilibria and always operates in bistability (cf. [2]). Only the values of E_{21}^0, E_{21}^1 and E_{21}^2 change with respect to m.

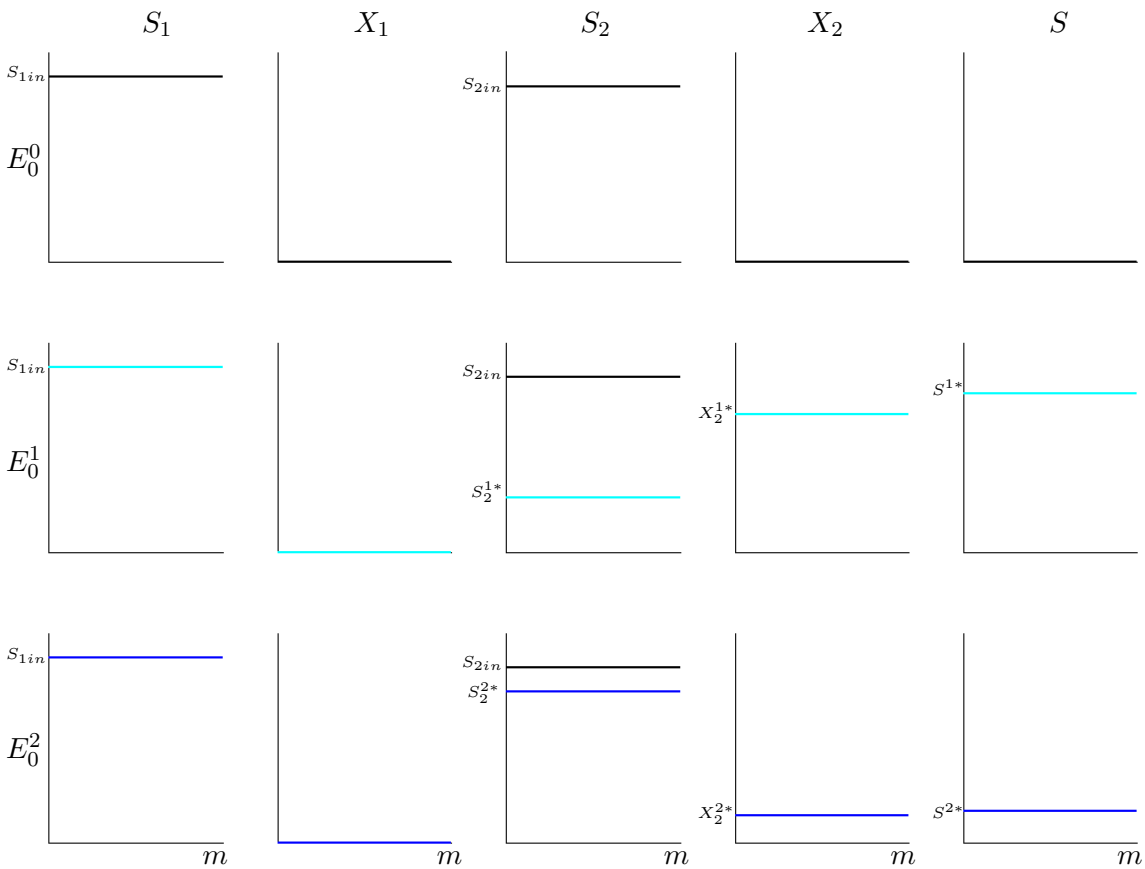

Figure 8: The components of the trivial equilibria E_0^0 (in black), E_0^1 (in cyan) and E_0^2 (in blue) in the Case A.

4.2. Generic Case B: Equilibria bifurcation for the AM2b, first example

We represent this case of operating conditions in Fig. 6. For $m = 0$, there is no intersection between the graph of $F_m(S)$ and the graphs of $G(S_1)$ and $H_i(S_1)$. Hence, there are no equilibria except washout equilibria E_0^0, E_1^1 and

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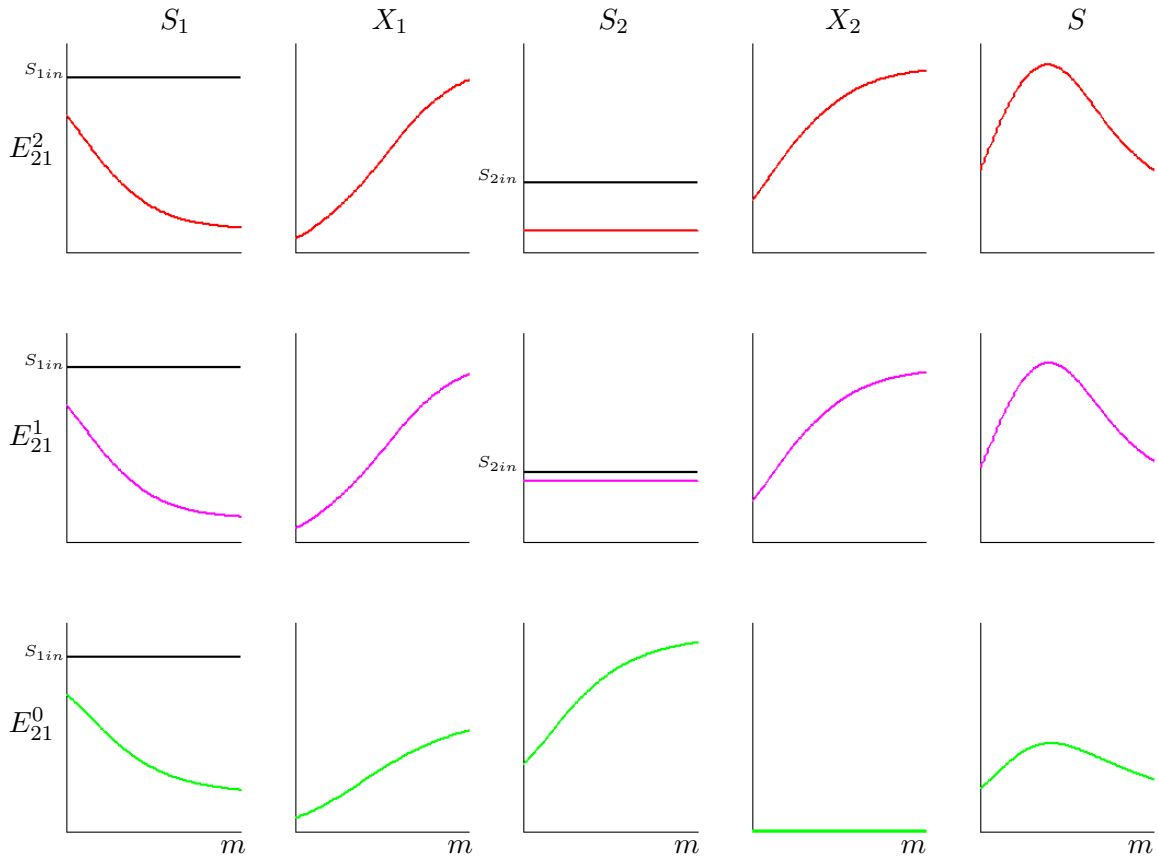

Figure 9: The components of the equilibrium points E_{21}^0 (in green), E_{21}^1 (in red) and E_{21}^2 (in magenta) in the case A.

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E_1^2, which do not depend on m and which exist if and only if (21) holds. If the value of m increases continuously, then the graph of $F_m(S)$ intersects first with the graphs of $H_1(S_1)$, then with the graph of $H_2(S_1)$ and finally with the graph of $G(S_1)$, in each case leading to the apparition of new equilibria. Let us use the following notations for the bifurcation values of m as it is illustrated in Fig. 10:

- $m = m_{c1}$: the value of m for the first intersection of F_m with H_1,
- $m = m_{c2}$: the value of m for the second intersection of F_m with H_2,
- $m = m_{c3}$: the value of m for the third intersection of F_m with G,
- $m = m_{c4}$: the value of m beyond which we have $S_{1in} = S_1^*$ for E_{22}^1 (the condition (26) becomes not satisfied and consequently E_{22}^1 passes to the gray area),
- $m = m_{c5}$: the value of m beyond which we have $S_{1in} = S_1^*$ for E_{22}^2 (the condition (26) becomes not satisfied and consequently E_{22}^2 passes to the gray area).

Each time when the value of m exceeds m_{ci}, $i = 1..5$, we have equilibria bifurcation. Thus, the system can have new equilibria or loose equilibria. More precisely, in Table 3 we give equilibria and their nature according to m, where T stands for *Trivial Equilibria*, $F_m \cap H_1$, $F_m \cap H_2$ and $F_m \cap G$ stand for *Equilibria obtained by the intersections of the graph* F_m *with graphs* H_1, H_2 *and* G, respectively, and S and U stand for a *Stable* and an *Unstable* Equilibrium, respectively. If there is no symbol, then it means that the equilibrium does not exist.

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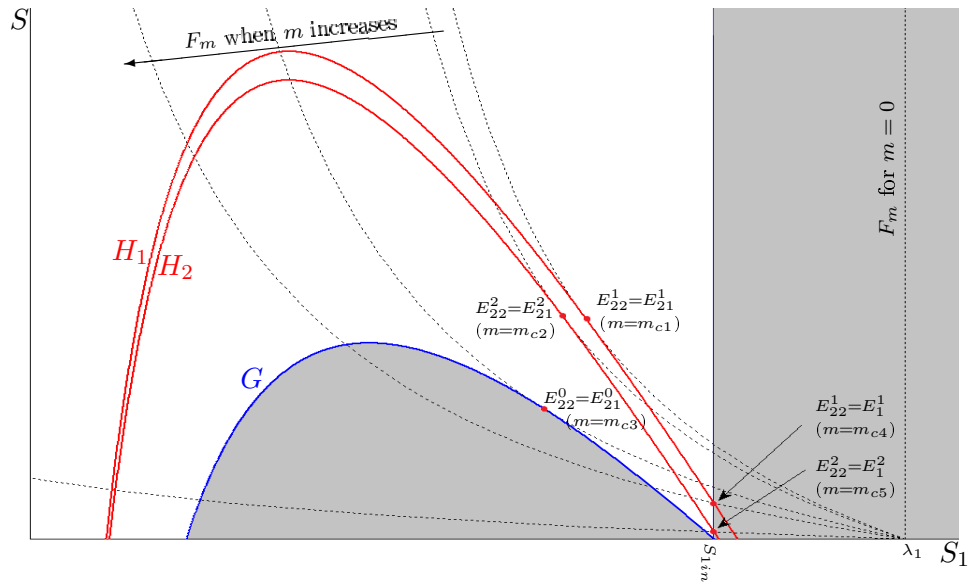

Figure 10: Values m_{ci}, $i = 1..5$ of m giving equilibria bifurcation in the generic case B.

Table 3: Equilibria and their nature in the generic case B represented in Fig. 6.

case B	Condition	Equilibria and nature								
		T			$F \cap G$		$F \cap H_1$		$F \cap H_2$	
		E^0_0	E^1_1	E^2_1	E^0_{21}	E^0_{22}	E^1_{21}	E^1_{22}	E^2_{21}	E^2_{22}
B.1	$0 \leq m < m_{c1}$	S	S	U						
B.2	$m_{c1} < m < m_{c2}$	S	S	U			S	U		
B.3	$m_{c2} < m < m_{c3}$	S	S	U			S	U	U	U
B.4	$m_{c3} < m < m_{c4}$	S	S	U	S	U	S	U	U	U
B.5	$m_{c4} < m < m_{c5}$	S	U	U	S	U	S		U	U
B.6	$m_{c5} < m$	S	U	U	S	U	S		U	

Here, with the parameter values used, the condition (21) is satisfied (see (32)). Thus, the system has generic bistability behavior if there is no intersection between F_m and H_i, $i = 1, 2$ and G as illustrated in case B.1 of Table 3. In case B.2, the system can have five equilibria of which three are

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locally stable (tristability behavior). In case B.3, we have seven equilibria, such that E_{21}^2 and E_{22}^2, obtained from the intersection of F_m with H_2, are both unstable. Under some operating conditions in case B.4, the system can have up to nine equilibria after the graph F_m intersects with the graph G. In this case, four equilibria are stable and the system exhibits quadristability behavior.

For some increasing values of m, the system can loose some equilibria. There are cases B.5 and B.6 of Table 3, when E_{22}^1 and E_{22}^2, respectively, pass into the gray area because henceforth condition (26) is not satisfied.

On the contrary to trivial equilibria E_0^0, E_1^1 and E_1^2, which do not depend on m, equilibria E_{2i}^0, E_{2i}^2 and E_{2i}^1, $i = 1, 2$ of Fig. 11 depend on m and can undergo bifurcation. For instance, we have the first bifurcation of E_{2i}^1 for $m = m_{c1}$. However, the equilibrium E_{22}^1 disappears later on for $m \geq m_{c4}$, because S_1^* becomes higher than S_{1in}. Equilibria E_{2i}^2 and E_{2i}^0 appear for $m = m_{c2}$ and $m = m_{c3}$ respectively.

In generic case B, the system (7)-(11) thus exhibits a rich qualitative behavior when the value of the bifurcation parameter m is changed. In particular, under some operating conditions (for $0 < m < m_{c1}$), the system AM2b (7)-(11) behaves exactly as the original system AM2 [2] and functions in bistability. However, under other operating conditions, when the value of m changes the system AM2b can have nine equilibria (for $m_{c3} < m < m_{c4}$) and functions in quadri-stability while for other values of m, it can function in tristability.

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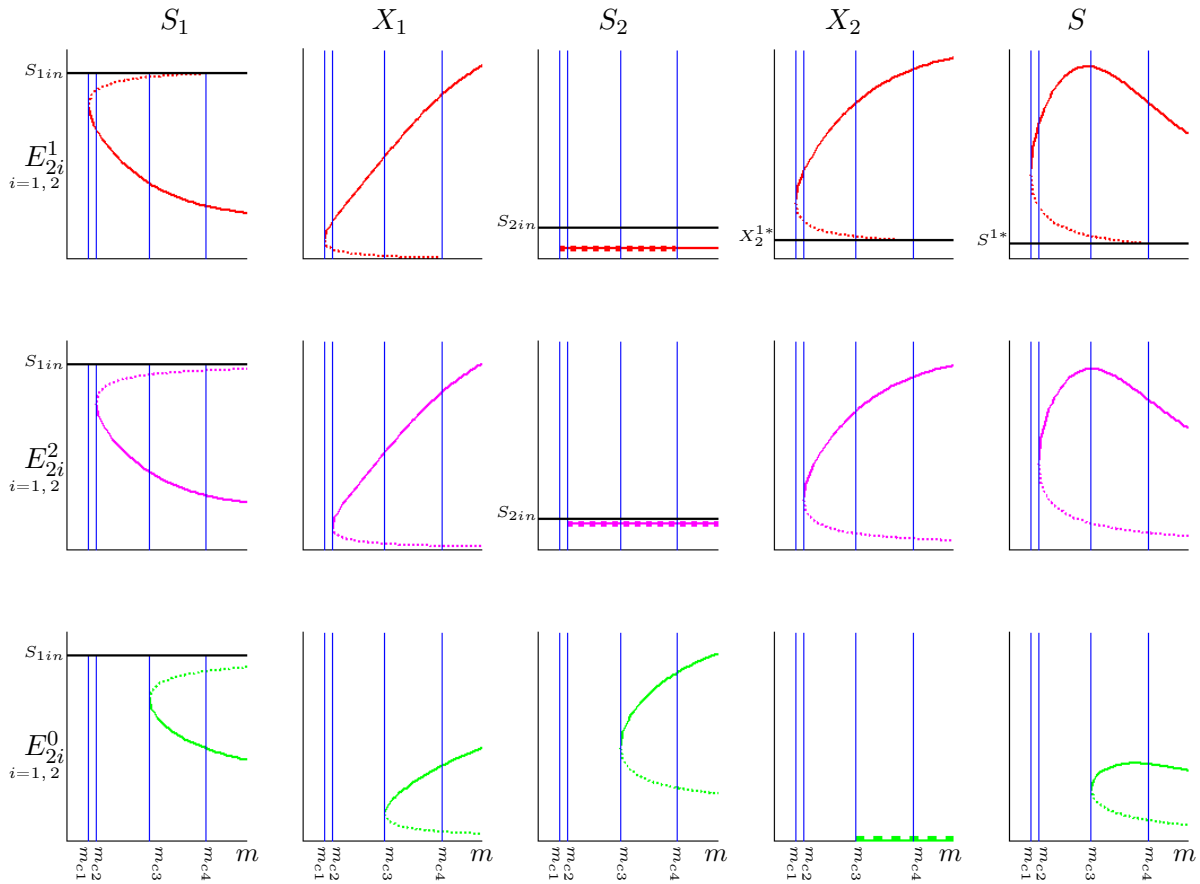

Figure 11: The components of the equilibrium points E^1_{21} (in solid red), E^1_{22} (in dash red), E^2_{21} (in solid magenta), E^2_{22} (in dash magenta), E^0_{21} (in solid green) and E^0_{22} (in dash green) in case B. The vertical lines correspond to the bifurcation values of m_{c1}, m_{c2}, m_{c3} and m_{c4}. The bifurcation value m_{c5}, for which the component S^*_1 of E^2_{22} is equal to S_{1in}, is too large and is not shown on the figure.

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4.3. Generic Case C: Equilibria bifurcation for the AM2b, second example

To illustrate the richness of the possible qualitative behavior of the AM2b model, we present in this section the generic case C, which is is described by Fig. 7. As shown previously in the generic case B, the system can have only the washout equilibira for $m = 0$, because there is no intersection between $F_m(S)$, $G(S_1)$ and $H_i(S_1)$, $i = 1, 2$. Washout equilibria exist if and only if condition (21) is verified. Here, in this generic case, we have:

$$S_2^{1*} = 0.0.1652 < S_{2in} = 0.6 < S_2^{2*} = 1.6348 \tag{33}$$

The equilibrium does not exist since $S_2^{2*} > S_{2in}$. The system has two washout equilibria E_0^0 and E_1^1. If the value of m increases, then we have intersections between $F_m(S)$ and $G(S_1)$ and $H_i(S_1)$, $i = 1, 2$ and, thus, equilibria bifurcation are obtained as illustrated in Fig. 12.

Beyond $m = m_{c4}$ (see Fig. 12), there is a large bifurcation, where $H_2(S_1^*) < G(S_1^*)$ for E_{22}^2. Henceforth, the condition (31) is not satisfied and the equilibrium E_{22}^2 disappears in the gray area. The equilibria and their nature are given in Table 4. The system can have two equilibria for $m < m_{c1}$ (see case C.1). Later on, it acquires new equilibria for $m_{c1} < m < m_{c4}$ (see cases C.2-C.4), or losses equilibria for $m > m_{c4}$ (see cases C.5-C.6). Notice that in case C.4, it has eight equilibria and functions in tristability (E_1^1, E_{21}^0 and E_{21}^1 are locally stable).

In Fig. 13, we present equilibria E_{2j}^0, E_{2j}^1 and E_{2j}^2, $i = 1, 2$.

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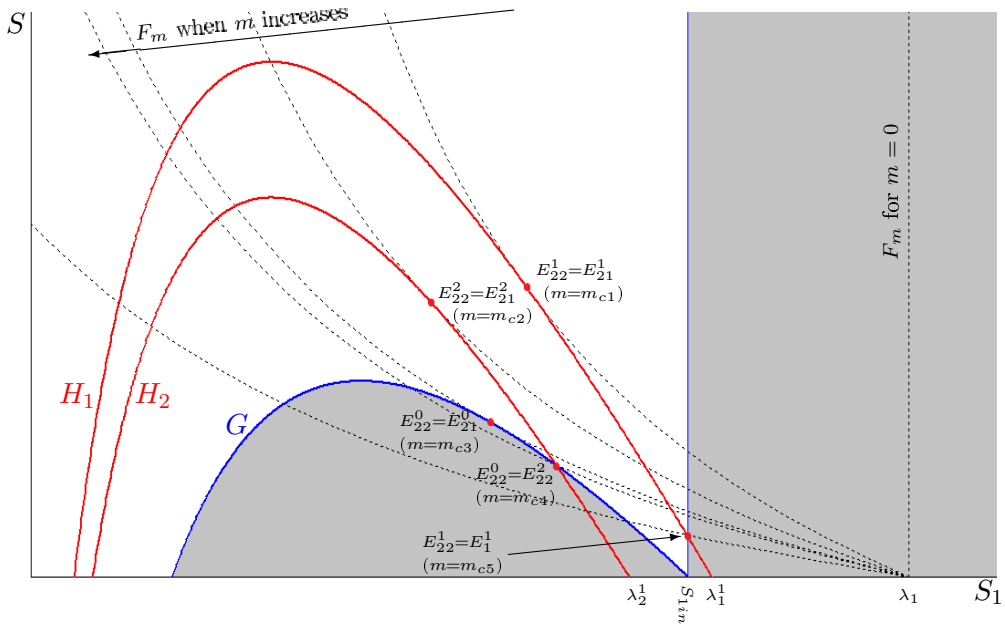

Figure 12: Values m_{ci}, $i = 1..5$ of m giving equilibria bifurcation in the generic case C.

Table 4: Equilibria and their nature in generic case C represented in Fig. 7. S and U have the same signification as in Table 3.

case C	Condition	Equilibria and nature							
		T		$F \cap G$		$F \cap H_1$		$F \cap H_2$	
		E^0_0	E^1_1	E^0_{21}	E^0_{22}	E^1_{21}	E^1_{22}	E^2_{21}	E^2_{22}
C.1	$0 \leq m < m_{c1}$	U	S						
C.2	$m_{c1} < m < m_{c2}$	U	S			S	U		
C.3	$m_{c2} < m < m_{c3}$	U	S			S	U	U	U
C.4	$m_{c3} < m < m_{c4}$	U	S	S	U	S	U	U	U
C.5	$m_{c4} < m < m_{c5}$	U	S	S	U	S	U	U	
C.6	$m_{c5} < m$	U	U	S	U	S		U	

4.4. Qualitative difference between AM2 and AM2b models

We have shown that models AM2 and AM2b may show significantly different qualitative behavior depending on model parameters and operating

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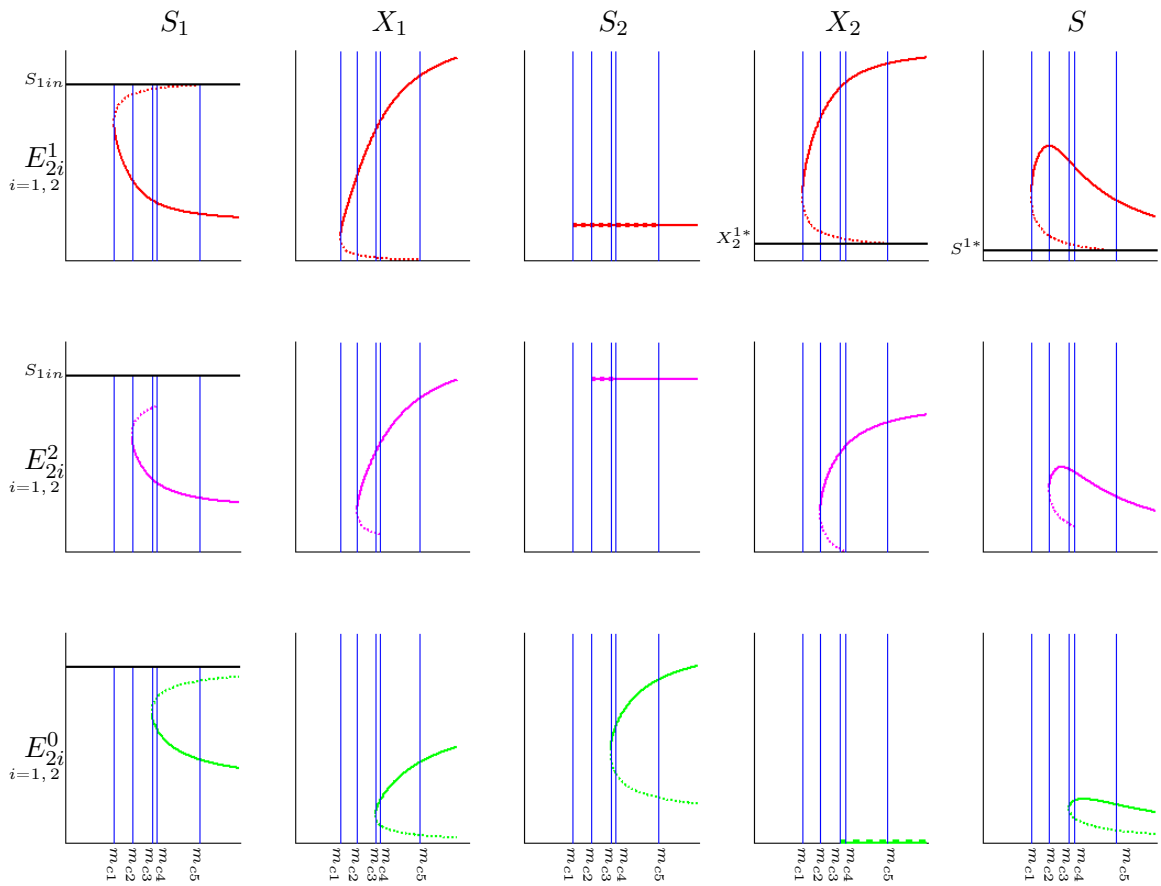

Figure 13: The components of the equilibrium points E^1_{21} (in solid red), E^1_{22} (in dash red), E^2_{21} (in solid magenta), E^2_{22} (in dash magenta), E^0_{21} (in solid green) and E^0_{22} (in dash green) in case C. The vertical lines correspond to the bifurcation values of m_{c1}, m_{c2}, m_{c3}, m_{c4} and m_{c5}.

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conditions. In particular, the steady-state value of the substrate concentration S_1 (denoted S_1^*) is not affected by the input substrate concentration S_{1in} in the AM2 or, to put it differently, in the AM2b with $m = 0$. When m differs from 0, it should be noted that the steady-state value of S_1 changes with S_{1in}. More precisely, S_1^* is a decreasing function of S_{1in} (cf. Fig. 14, the intersection between curves F_m and H_1 when S_{1in} increases and Fig. 15).

This important qualitative difference between the AM2 and the AM2b models can be used for modeling purposes in order to validate this new model in the following way: assuming we have access to steady-state data, we need only to look at the different steady-states obtained with different S_{1in} and compare the corresponding values of substrates S_1^*. If they differ, AM2 is not a good candidate for modeling while AM2b can be used instead.

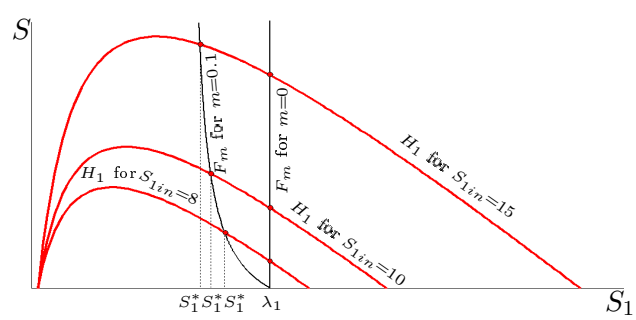

Figure 14: Modeling of the equilibrium S_1^* with the model AM2b when S_{1in} changes. Here, $K_1 = 10$, $S_2 = 0.6$, $D_1 = 0.25$, $m = 0 - 1$ and $S_{1in} = 8 - 10 - 15$. Other parameters values are those given in Table 1.

5. Conclusion

In this paper, we have developed and studied a mathematical model for an AnMBR. The new model, named AM2b, was developed by modifying the

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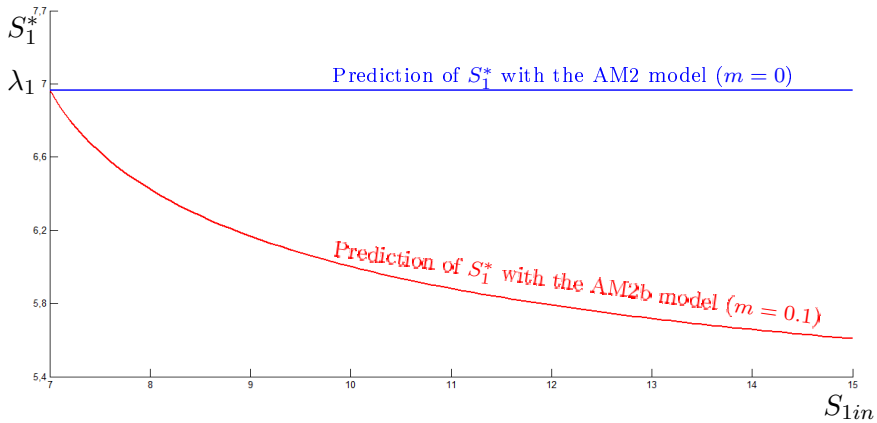

Figure 15: Evolution of the equilibrium S_1^* according to S_{1in} for $m = 0$ and $m = 0.1$. Parameter values used are the same as in Fig. 14.

AM2 model [1] to integrate SMP production and degradation. The mass balance equations are proposed in considering a new reaction network taking into account certain assumptions about the functioning of the AnMBR, in particular the behavior of the different variables with respect to the presence of a membrane. A graph-based approach to study the developed model has been presented and illustrated by numerical simulations. We studied three generic cases of system behavior in the light of the values of the relevant biological parameters, in particular the maximum growth rate m of acidogenic bacteria on SMP. We show that in one of these cases, the AM2b system behaves exactly like the AM2 system. It always operates in bistability for all value of m. However, in the two other generic cases, the system displays rich qualitative behavior and can have up to nine equilibria while showing multi-stability behavior. We also show that the AM2b system can predict the change of equilibrium S_1^* of the organic matter when the influent concentration S_{1in} changes.

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Perspectives for further work include: i) the design of observers to estimate biomasses X_1 and X_2, SMP and kinetics; ii) the validation of hypotheses to confront the AM2b model with experimental data; and iii) the coupling of this model with models of membrane modules in order to design hybrid models for the complete description of an AnMBR for use in process control.

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Abbreviations

MBR	Membrane BioReactor
$AnMBR$	Anaerobic Membrane BioReactor
SMP	Soluble Microbial Products
EPS	Extra-cellular Polymeric Substances
UAP	Utilization Associated Products
BAP	Biomass Associated Products
$WWTP$	Waste Water Treatment Plant
ASM	Activated Sludge Model
$AM2$	2-steps Acidogenesis - Methanogenesis model
$AM2b$	AM2 model with SMP dynamics
COD	Chemical Oxygen Demand
VFA	Volatile Fatty Acids

Nomenclature

X_1	concentration of acidogenic bacteria	$[g/l]$
X_2	concentration of methanogenic bacteria	$[g/l]$
S_1	concentration of organic matter	$[g/l]$
S_2	concentration of VFA	$[g/l]$
S_{1in}	the input concentration of S_1	$[g/l]$
S_{2in}	the input concentration of S_2	$[g/l]$
S	concentration of SMP	$[g/l]$
CH_4	produced methane	
CO_2	carbon dioxide	
k_1	yield of S_1 degradation by X_1	$[gCOD_{X_1}/gCOD_{S_1}]$
k_2	yield of S_2 production from S_1	$[gCOD_{S_2}/gCOD_{S_1}]$
k_3	yield of S_2 degradation by X_2	$[gCOD_{X_2}/gCOD_{S_2}]$
k_4	yield of CO_2 production from S_1	$[gCOD_{X_1}/gCOD_{S_1}]$
k_5	yield of CO_2 production from S_2	$[gCOD_{CO_2}/gCOD_{S_2}]$
k_6	yield of CH_4 production from S_2	$[gCOD_{CH_4}/gCOD_{S_2}]$
b_1	yield of SMP degradation by X_1	$[gCOD_{X_1}/gCOD_{SMP}]$
b_2	yield of S_2 production from SMP	$[gCOD_{S_2}/gCOD_{SMP}]$
b_3	yield of SMP production from S_1	$[gCOD_{SMP}/gCOD_{S_1}]$
b_4	yield of SMP production from S_2	$[gCOD_{SMP}/gCOD_{S_2}]$
β	SMP fraction leaving the bioreactor	
ΔP	transmembrane pressure	$[Pa]$
ΔP_{cri}	critic transmembrane pressure	$[Pa]$
J	membrane flux	$[L/(h.m^2)]$
J_{limite}	threshold membrane flux	$[L/(h.m^2)]$
J_{cri}	critic membrane flux	$[L/(h.m^2)]$

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The original publication is available at http://www.sciencedirect.com.
DOI : 10.1016/j.cej.2013.05.073

μ_1	acidogenesis kinetics	$[1/d]$
μ_2	methanogenesis kinetics	$[1/d]$
μ	kinetic of SMP degradation	$[1/d]$
m_1	maximum acidogenic biomass growth rate on S_1	$[1/d]$
m_2	maximum methanogenic biomass growth rate on S_2	$[1/d]$
m	maximum acidogenic biomass growth rate on S	$[1/d]$
K_1	half-saturation constant associated with S_1	$[g/L]$
K_2	half-saturation constant associated with S_2	$[g/L]$
K_i	inhibition constant associated with S_2	$[g/L]$
K	half-saturation constant associated with S	$[g/L]$
Q_{in}	the input flow of the bioreactor	$[L/d]$
Q_{out}	the output flow of the bioreactor	$[L/d]$
Q_1	the withdraw flow from the bioreactor	$[L/d]$
V	the volume of the bioreactor	$[L]$
D	the dilution rate	$[1/d]$
D_0	the decay rate of biomasses	$[1/d]$
D_1	the biomass withdraw	$[1/d]$
ξ^*	the value of the component ξ at equilibrium ($\xi = S_1$, X_1, S_2, X_1 or S)	
E^*, E_{2i}^j	equilibria, $i = 1, 2$, $j = 0, 1, 2$	

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