Tunis meeting, November 2010

TREASURE Project (Treatment and Sustainable Reuse of Effluents in semiarid climates)

FROM THE AM2 MODEL TO THE AM2b MODEL: DEVELOPMENT AND MATHEMATICAL ANALYSIS

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Theme : Modeling and control of membranes bioreactors

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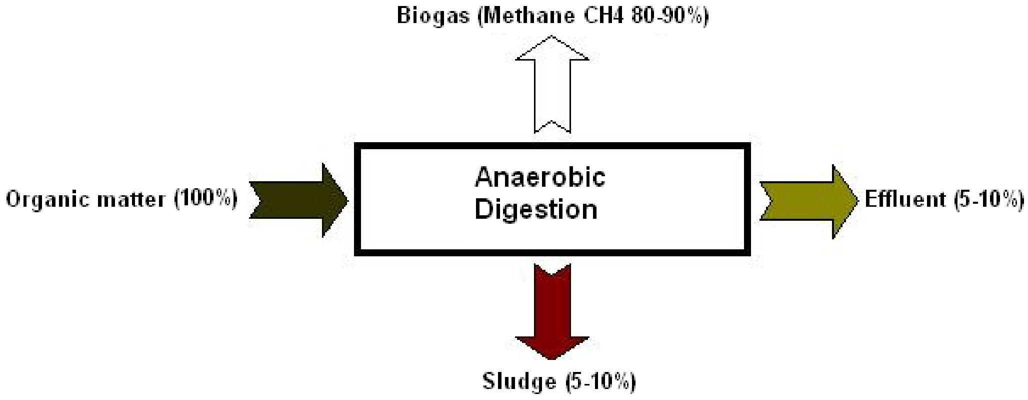
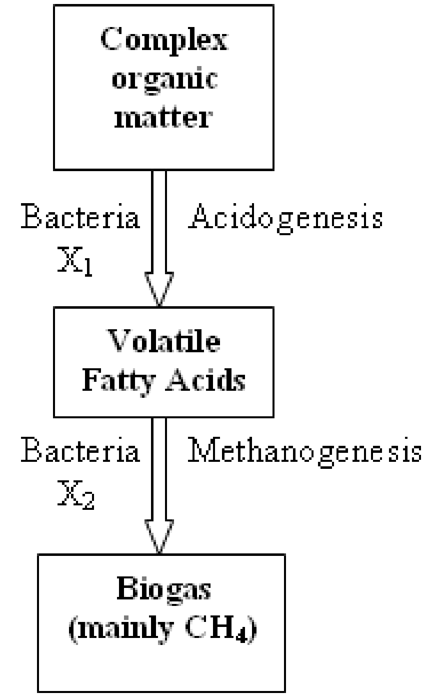
Outline of the presentation:

- Equilibria of the AM2 model (AMOCO[(*)] model)
- Development of the AM2b model
- Mathematical analysis of the AM2b Model.
- Numerical simulations and discussions.
- Conclusions.

(*) **A**dvanced **MO**nitoring and **CO**ntrol system for anaerobic process, European FAIR project N ERB-FAIR-CT961198

Anaerobic Digestion:





The Anaerobic Digestion is based on 2 main reactions

Acidogenesis : $S_1 \rightarrow X_1 + S_2 + CO_2$

Methanogenesis : $S_2 \rightarrow X_2 + CH_4 + CO_2$

However, this process can be unstable, because of accumulation of Volatile Fatty Acids (AGV), noted S_2 in the model (acidification of the bioreactor)

Anaerobic Digestion Model (AMOCO Model):

ADM1 (Anaerobic Digestion Model 1) developed by IWA : Full model BUT complex !!

➔ Simplified model : AMOCO(*) Model or AM2 Model

$$\begin{cases} \dot{S}_1 = D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1 & (1) \\ \dot{X}_1 = (\mu_1(S_1) - \alpha D)X_1 & (2) \\ \dot{S}_2 = D(S_{2in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 & (3) \\ \dot{X}_2 = (\mu_2(S_2) - \alpha D)X_2 & (4) \end{cases}$$

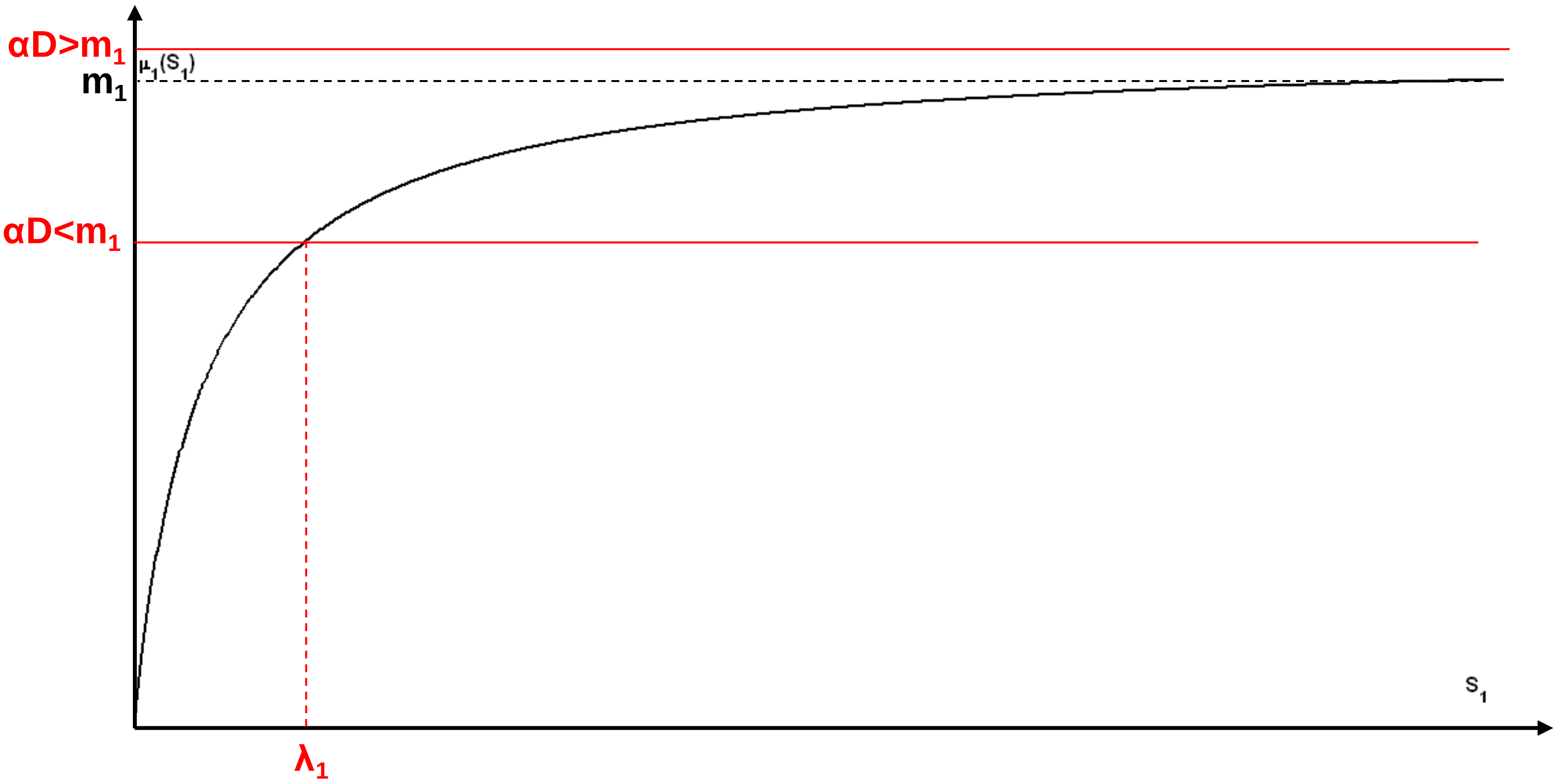
At steady state, we have from (2) and (4) :

$$X_1 = 0 \ or \ \mu_1(S_1) = \alpha D$$

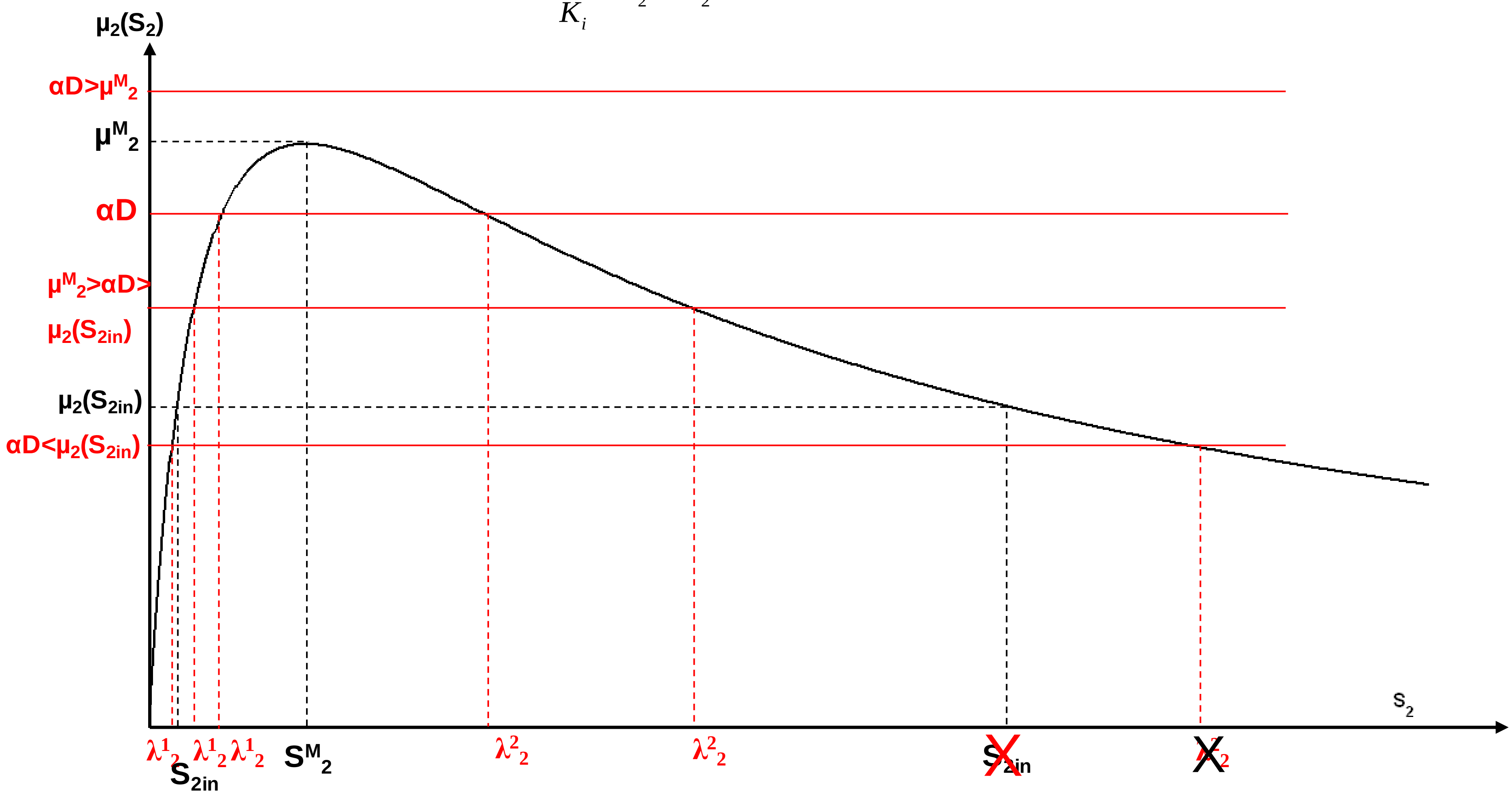
$$X_2 = 0 \ or \ \mu_2(S_2) = \alpha D$$

Case where $\mu_1(S_1)$ is of Monod type

$$\mu_1(S_1) = \frac{m_1 S_1}{K_1 + S_1}$$



$\mu_2(S_2)$ is Haldane type $\mu_2(S_2) = \dfrac{m_2 S_2}{\dfrac{S_2^2}{K_i} + S_2 + K_2}$ S_{2in} : the total influent concentration of S_2



S_{2in}^{*} : the true concentration of S_2 available for the methanogenesis reaction

S_{1in}

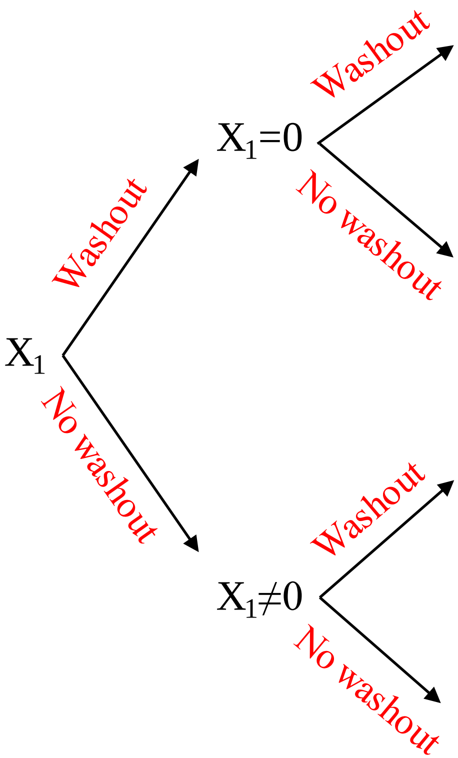
$$\begin{aligned} \dot{S}_1 &= D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1 \\ \dot{X}_1 &= [\mu_1(S_1) - \alpha D]X_1 \end{aligned}$$

$$\frac{k_2}{k_1}(S_{1in} - \lambda_1) + S_{2in} = S_{2in}^{*}$$

$$\begin{aligned} \dot{S}_2 &= D(S_{2in} - S_2) + k_2\mu_1(S_1)X_1 - k_3\mu_2(S_2)X_2 \\ \dot{X}_2 &= [\mu_2(S_2) - \alpha D]X_2 \end{aligned}$$

We can see the system like a cascade of two sub-systems. For that, we must have a good a-priori knowledge about the whole parameters and inputs of reactor. In particular, we must be able to characterize the true concentration of S_2 in input of the methanogenesis.

The system (1-4) has at most six equilibrium points:



$X_2=0 \Rightarrow E_1^0 = (S_{1in}, 0, S_{2in}, 0)$

which always exists

$X_2 \neq 0 \Rightarrow E_1^i = (S_{1in}, 0, \lambda_2^i, X_2^i)$ où $X_2^i = \frac{1}{k_3 \alpha}(S_{2in} - \lambda_2^i),\ i = 1,2$

which exists if and only if $S_{2in} > \lambda_2^i$

$X_2=0 \Rightarrow E_2^0 = (\lambda_1, X_1^*, S_{2in}^*, 0)$ où $X_1^* = \frac{1}{k_1 \alpha}(S_{1in} - \lambda_1)$

which exists if and only if $S_{1in} > \lambda_1$

$X_2 \neq 0 \Rightarrow E_2^i = (\lambda_1, X_1^*, \lambda_2^i, X_2^{i*})$ où $X_2^{i*} = \frac{1}{k_3 \alpha}(S_{2in}^* - \lambda_2^i),\ i = 1,2$

which exists if and only if $S_{1in} > \lambda_1$ *and* $S_{2in}^* > \lambda_2^i$

Existence and stability of the hyperbolic equilibria :

If there is washout of X_1 then we have 3 equilibria

1	$S_{1in} < \lambda_1$	E_1^0	E_1^1	E_1^2
1.1	$S_{2in} < \lambda_2^1$	S		
1.2	$\lambda_2^1 < S_{2in} < \lambda_2^2$	I	S	
1.3	$\lambda_2^2 < S_{2in}$	S	S	I

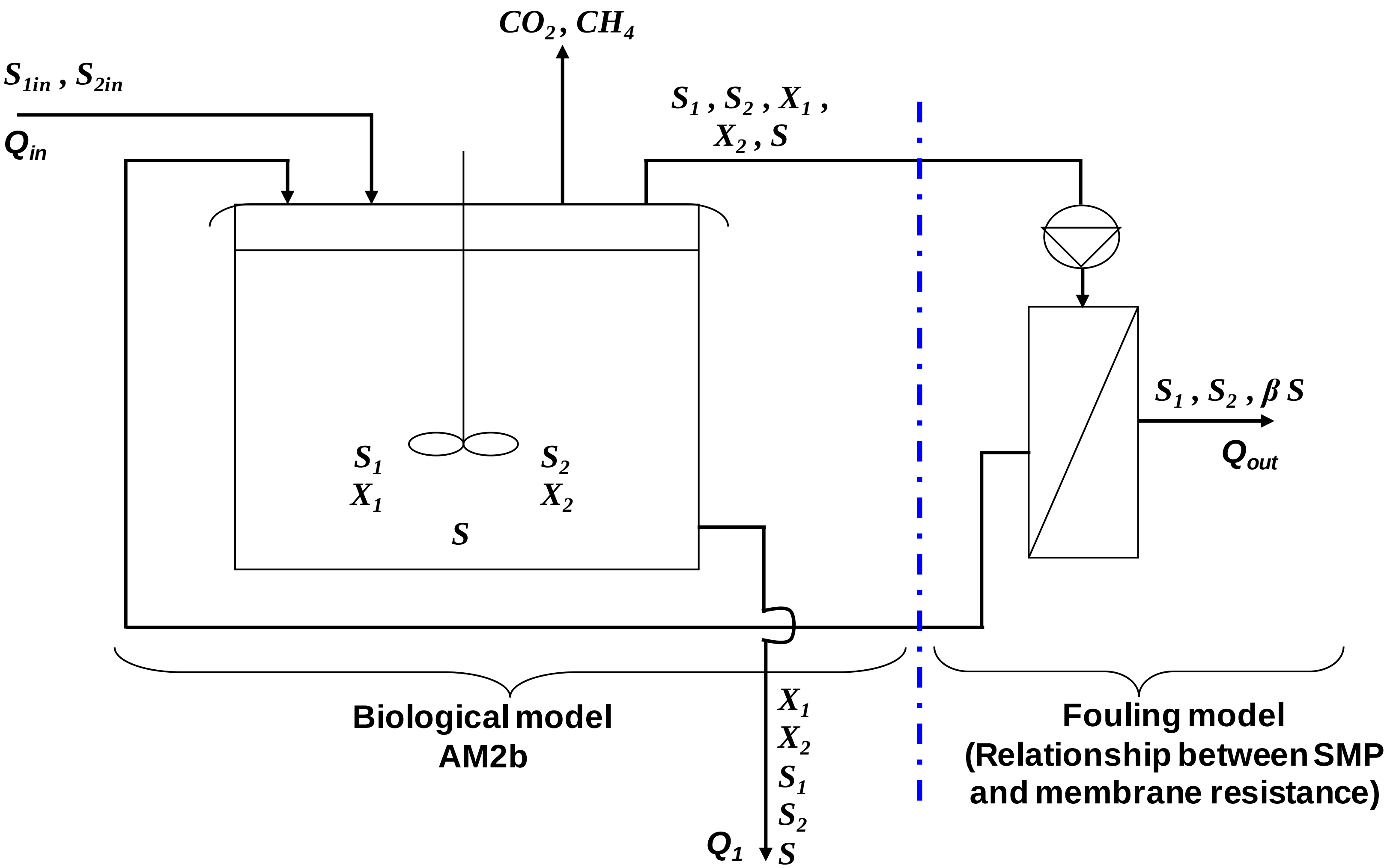
If $\lambda_1 < S_{1in}$ we denote by:

$$S_{2in}^* = S_{2in} + \frac{k_2}{D}\mu_1(S_1^*)X_1^* = S_{2in} + \frac{k_2}{k_1}(S_{1in} - \lambda_1)$$

If there is no washout of X_1 then we have 6 equilibria

2	$S_{1in} > \lambda_1$	E_1^0	E_1^1	E_1^2	E_2^0	E_2^1	E_2^2
2.1	$S_{2in}^* < \lambda_2^1$	I			S		
2.2	$S_{2in} < \lambda_2^1 < S_{2in}^* < \lambda_2^2$	I			I	S	
2.3	$S_{2in} < \lambda_2^1 < \lambda_2^2 < S_{2in}^*$	I			S	S	I
2.4	$\lambda_2^1 < S_{2in} < S_{2in}^* < \lambda_2^2$	I	I		I	S	
2.5	$\lambda_2^1 < S_{2in} < \lambda_2^2 < S_{2in}^*$	I	I		S	S	I
2.6	$\lambda_2^1 < \lambda_2^2 < S_{2in}$	I	I	I	S	S	I

AM2 … toward the AM2b model



Hypotheses for the model development

H1. The reactional medium of the bioreactor is considered to be a homogeneous.

H2. The substrates S_1 and S_2 cross the external membrane without retention (the molecules size is smaller than the pore diameter).

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

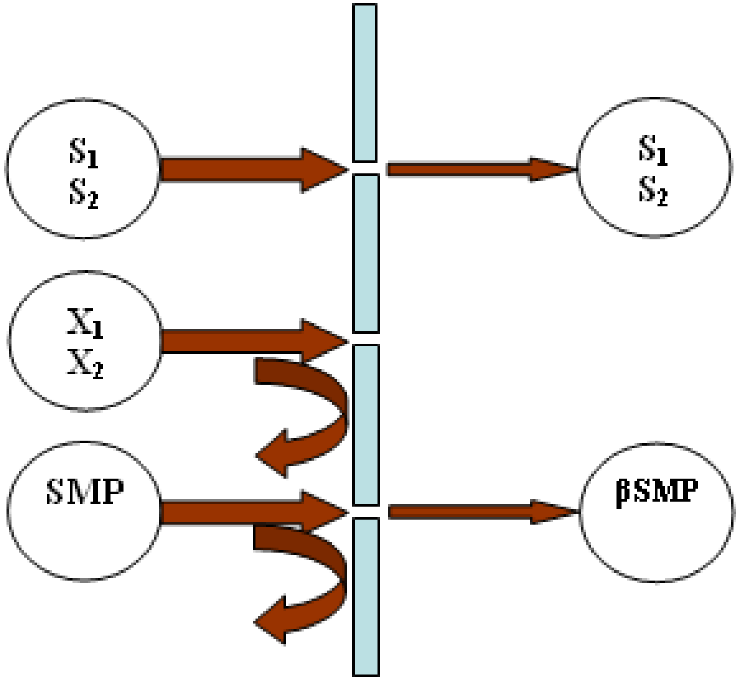
H4. Decay rates D_0 of biomasses are taken into account.

H5. The withdraw of the biomass with a flowrate Q_1 is considered.

H6. $SMP = UAP + BAP$ are grouped into an unique variable of concentration S, which only a fraction β leaves the bioreactor. The remaining, corresponding to macromolecules, is retained by the membrane. This is modeled in the mass balance equation by $-\beta DS$ where $0 \leq \beta \leq 1$ ($\beta=0$: total retention of *SMP* by the membrane; $\beta=1$: free crossing of *SMP* through the membrane).

H7. The bioreactor is supposed to operate in normal conditions (no critical fouling: the flux is lower than the critical flux).

Matter separation by the membrane:



Reaction schemes and mathematical equations

The reaction schemes of the model AM2 are:

i- Acidogenesis : $k_1 S_1 \rightarrow X_1 + k_2 S_2 + k_4 CO_2$

ii- Methanogenesis : $k_3 S_2 \rightarrow X_2 + k_5 CH_4 + k_6 CO_2$

We model the *SMP* production from the degradation of S_1, S_2 and the decay of biomasses X_i. In addition, we consider the *SMP* degradation into S_2, CH_4 and CO_2 through the growth of X_1.

i- Acidogenesis + *SMP* Production:

$$k_1 S_1 \rightarrow X_1 + k_2 S_2 + b_3 S + k_4 CO_2$$

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

ii- Methanogenesis + *SMP* Production:

$$k_3 S_2 \rightarrow X_2 + b_4 S + k_5 CO_2 + k_6 CH_4$$

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

iii- *SMP* Degradation:

$$b_1 S \rightarrow X_1 + b_2 S_2 + k_7 CO_2 + k_8 CH_4$$

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

iv- *SMP* Production from biomass decay:

$$X_1 \rightarrow D_0 S, \quad X_2 \rightarrow D_0 S$$

We note ξ the state space vector of the new model AM2b:

$$\xi = [S_1, X_1, S_2, X_2, S]$$

The mathematical model is:

$$\begin{cases} \dot{S}_1 = D(S_{1in} - S_1) - k_1\mu_1(S_1)X_1 & (1) \\ \dot{X}_1 = [\mu_1(S_1) + \mu(S) - D_0 - D_1]X_1 & (2) \\ \dot{S}_2 = D(S_{2in} - S_2) - k_3\mu_2(S_2)X_2 + [k_2\mu_1(S_1) + b_2\mu(S)]X_1 & (3) \\ \dot{X}_2 = [\mu_2(S_2) - D_0 - D_1]X_2 & (4) \\ \dot{S} = [b_3\mu_1(S_1) + D_0 - b_1\mu(S)]X_1 + [b_4\mu_2(S_2) + D_0]X_2 - [\beta D + (1-\beta)D_1]S & (5) \end{cases}$$

k_i and b_i: the stochiometric coefficients.

D_0: decay rate of biomass.

D_1: withdraw of biomass.

D: dilution rate.

β: SMP fraction leaving the bioreactor.

Model equilibria: The characteristics of the kinetics μ_1, μ_2 and μ are

- $\mu_1(0) = \mu_2(0) = \mu(0) = 0$
- $\mu_1'(S_1) > 0 \text{ for } S_1 \geq 0 \text{ and } \mu'(S) > 0 \text{ for } S \geq 0$
- $\mu_1(\infty) = m_1 \text{ and } \mu(\infty) = m$
- $\mu_2'(S_2) > 0 \text{ if } 0 \leq S_2 \leq S_2^M$
- $\mu_2(S_2^M) = \mu_S^M$
- $\mu_2'(S_2) < 0 \text{ if } S_2 > S_2^M$

As examples:

$$\mu_1(S_1) = \frac{m_1 S_1}{K_1 + S_1}, \qquad \mu_2(S_2) = \frac{m_2 S_2}{\frac{S_2^2}{K_I} + S_2 + K_2}, \qquad \mu(S) = \frac{mS}{K + S}$$

To compute equilibrium points, we cancel (1) to (5):

$$(2)=0 \Leftrightarrow [\mu_1(S_1)+\mu(S)-D_0-D_1]X_1=0$$

$$\Rightarrow X_1=0$$

$$\Rightarrow [\mu_1(S_1)+\mu(S)-D_0-D_1]=0$$

$$(4)=0 \Leftrightarrow [\mu_2(S_2)-D_0-D_1]X_2=0$$

$$\Rightarrow X_2=0$$

$$\Rightarrow [\mu_2(S_2)-D_0-D_1]=0$$

We consider three cases:

1. $X_1=0$
2. $X_1>0$ and $X_2=0$
3. $X_1>0$ and $X_2>0$

Lemma . The equilibria (S_1, X_1, S_2, X_2, S) of the system (1-5) 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, $E_0^i = (S_{1in}, 0, \lambda_2^i, X_2^i, S^{i*})$, $i = 1$ or 2, where

$$X_2^i = \frac{D(S_{2in} - \lambda_2^i)}{k_3(D_0 + D_1)},$$

$$S^{i*} = \frac{b_4 + \frac{D_0}{D_0+D_1}}{[\beta + (1-\beta)\frac{D_1}{D}]k_3}(S_{2in} - \lambda_2^i), \qquad i = 1, 2$$

Which exists if and only if $S_{2in} > \lambda_2^i$.

Lemma . Let (X_1, X_2, S_1, S_2, S) an equilibrium point of system (1-5). If $X_1 > 0$ and $X_2 = 0$ then one has $0 < S_1 < S_{1in}$, $S > 0$ and $S_2 > 0$. Moreover S_1 and S are solutions of equations $S_1 = F(S)$ and $S = G(S_1)$ and X_1 and S_2 are given by the formulas

$$X_1 = D\frac{S_{1in} - S_1}{k_1\mu_1},$$

$$S_2 = S_{2in} + [k_2\mu_1 + b_2\mu]\frac{S_{1in} - S_1}{k_1\mu_1}.$$

Such that:

$$F(S) := \mu_1^{-1}(D_0 + D_1 - \mu(S))$$

$$G(S_1) := \frac{1}{B}[S_{1in} - S_1][\frac{1}{k_1}(b_3 + b_1) + \frac{1}{k_1\mu_1}(D_0 - b_1(D_1 + D_0))]$$

$$B = \beta + (1 - \beta)\frac{D_1}{D}$$

Lemma . Let (X_1, X_2, S_1, S_2, S) an equilibrium point of system (1-5). If $X_1 > 0$ and $X_2 > 0$ then one has $0 < S_1 < S_{1in}$, $S > 0$ and $S_2 = \lambda_2^i$. Moreover S_1 and S are solutions of equations $S_1 = F(S)$ and $S = H_i(S_1)$ and X_1 and X_2 are given by the formulas

$$X_1 = D\frac{S_{1in} - S_1}{k_1\mu_1}.$$

$$X_2 = D\frac{[S_{1in} - S_1][k_2\mu_1 + b_2\mu] + (S_{2in} - \lambda_2^i)k_1\mu_1}{k_1k_3(D_0 + D_1)\mu_1}.$$

With the following condition:

$$\lambda_2^i < S_{2in} + (k_2\mu_1 + b_2\mu)\frac{S_{1in} - S_1}{k_1\mu_1}.$$

Such that:

$$H_i(S_1) := \frac{1}{B}[A(S_{2in} - \lambda_2^i) + (S_{1in} - S_1)(\frac{A_1 - A_2}{k_1} + \frac{A_2(D_1 + D_0) + D_0}{k_1\mu_1})], \qquad i = 1, 2$$

$S_2 = \lambda_2^i$ is a solution of equation $\mu_2(S_2) = D_0 + D_1$

Graphic calculation of equilibria

The equilibrium points are obtained from the intersection of the graph of

$$F(S) := \mu_1^{-1}(D_0 + D_1 - \mu(S))$$

With the graphs of

$$G(S_1) := \frac{1}{B}[S_{1in} - S_1][\frac{1}{k_1}(b_3 + b_1) + \frac{1}{k_1\mu_1}(D_0 - b_1(D_1 + D_0))]$$

$$H_i(S_1) := \frac{1}{B}[A(S_{2in} - \lambda_2^i) + (S_{1in} - S_1)(\frac{A_1 - A_2}{k_1} + \frac{A_2(D_1 + D_0) + D_0}{k_1\mu_1})], \quad i = 1, 2$$

The function *F* depends on *μ(S*), it changes the form according to the value of *m*.

The functions *G, H_1* and *H_2* do not depend on the kinetic *μ(S)*, but depend on the others parameters.

$$k_1S_1 \rightarrow X_1 + k_2S_2 + b_3S + k_4CO_2$$
$$k_3S_2 \rightarrow X_2 + b_4S + k_5CO_2 + k_6CH_4$$
$$b_1S \rightarrow X_1 + b_2S_2 + k_7CO_2 + k_8CH_4$$

From the biological mass balance principle:

The quantity of biomass and products produced is always smaller than the quantity of substrate consumed.

$k_1 \geq 1 + b_3 + k_2$

$k_3 \geq 1 + b_4$

$b_1 \geq 1 + b_2$

SMP are slowly produced and degraded in the bioreactor.

$k_1 > b_1$: The degraded quantity S of SMP is smaller than the degraded quantity S_1 of substrate.

$k_2 > b_2$: The produced quantity S_2 of VFA from S_1 is higher than the produced quantity from the SMP.

$k_2 > b_3$: The produced quantity S_2 of VFA from S_1 is higher than the produced quantity S of SMP from S_1.

$b_4 < k_1, k_2, k_3$: The produced quantity S of SMP from S_2 is small, the most part of S_2 is converted in biogas.

Simulation results:

Idea : look at the equilibria bifurcation according to the value of *m*.

Table 1. Nominal parameters values

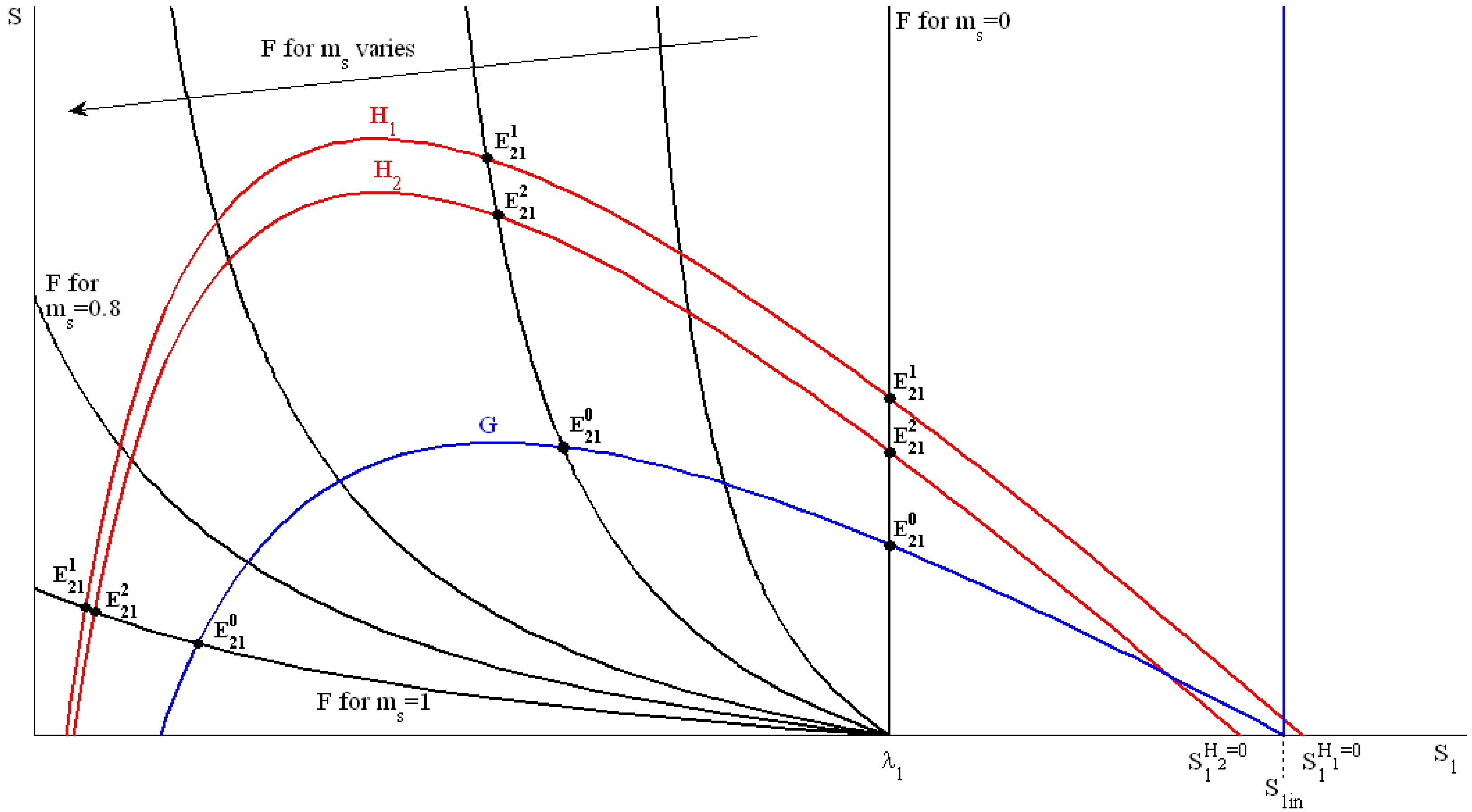
Parameters	Nominal values	Parameters	Nominal values
m_1	1.2	k_3	268
K_1	change	b_1	5
m_2	1.5	b_2	10
K_2	5	b_3	7
K_I	15	b_4	5
β	0.6	m	[0..1]
k_1	25	K	3
k_2	250		

The values of the operating parameters are.

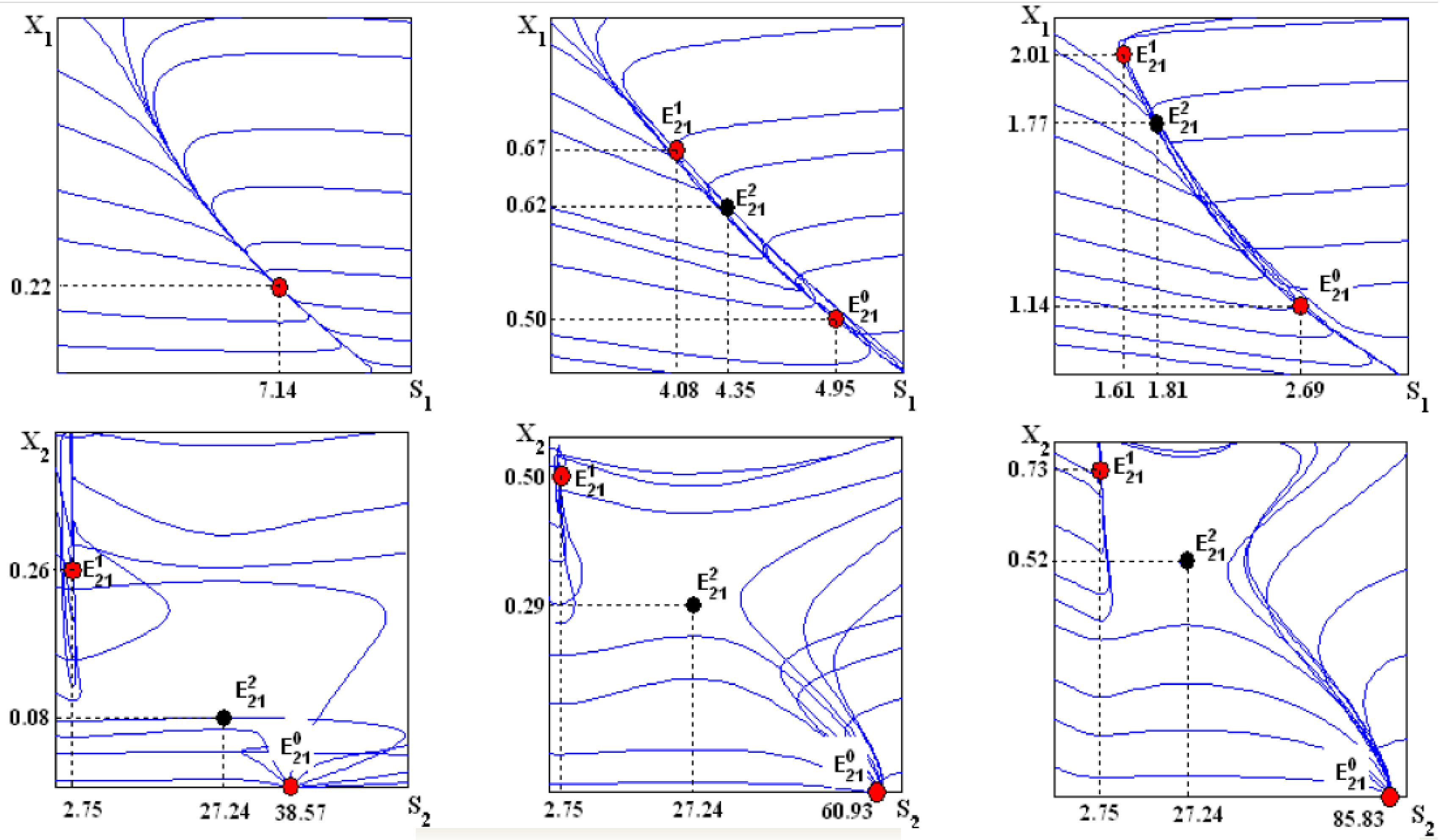
$$D = 1, D_0 = 0.25, D_1 = 0.25, S_{1in} = 10, S_{2in} = 10$$

Case 1: $\lambda_1 < S_1^{H_2=0} < S_{1in} < S_1^{H_1=0}$

We focus our study on the case, where we have always three equilibrium points as in case of the model AM2.



Phase planes:



Equilibria stability:

We calculated the Jacobian of system: $Jac = \frac{\partial f}{\partial \xi}$

We replaced equilibria by their numerical values.

We calculated the eigenvalues for each equilibrium.

Theorem. If there is no washout of X_1 then the system has three equilibria:

- $E_{21}^{1} = (\lambda_{21}^{1}, X_{1,21}^{1}, \lambda_{2}^{1}, X_{2,21}^{1}, S_{21}^{1})$: Stable
- $E_{21}^{2} = (\lambda_{21}^{2}, X_{1,21}^{2}, \lambda_{2}^{2}, X_{2,21}^{2}, S_{21}^{2})$: Unstable
- $E_{21}^{0} = (\lambda_{21}^{0}, X_{1,21}^{0}, S_{2,21}^{0}, 0, S_{21}^{0})$: Stable

Conclusions drawn:

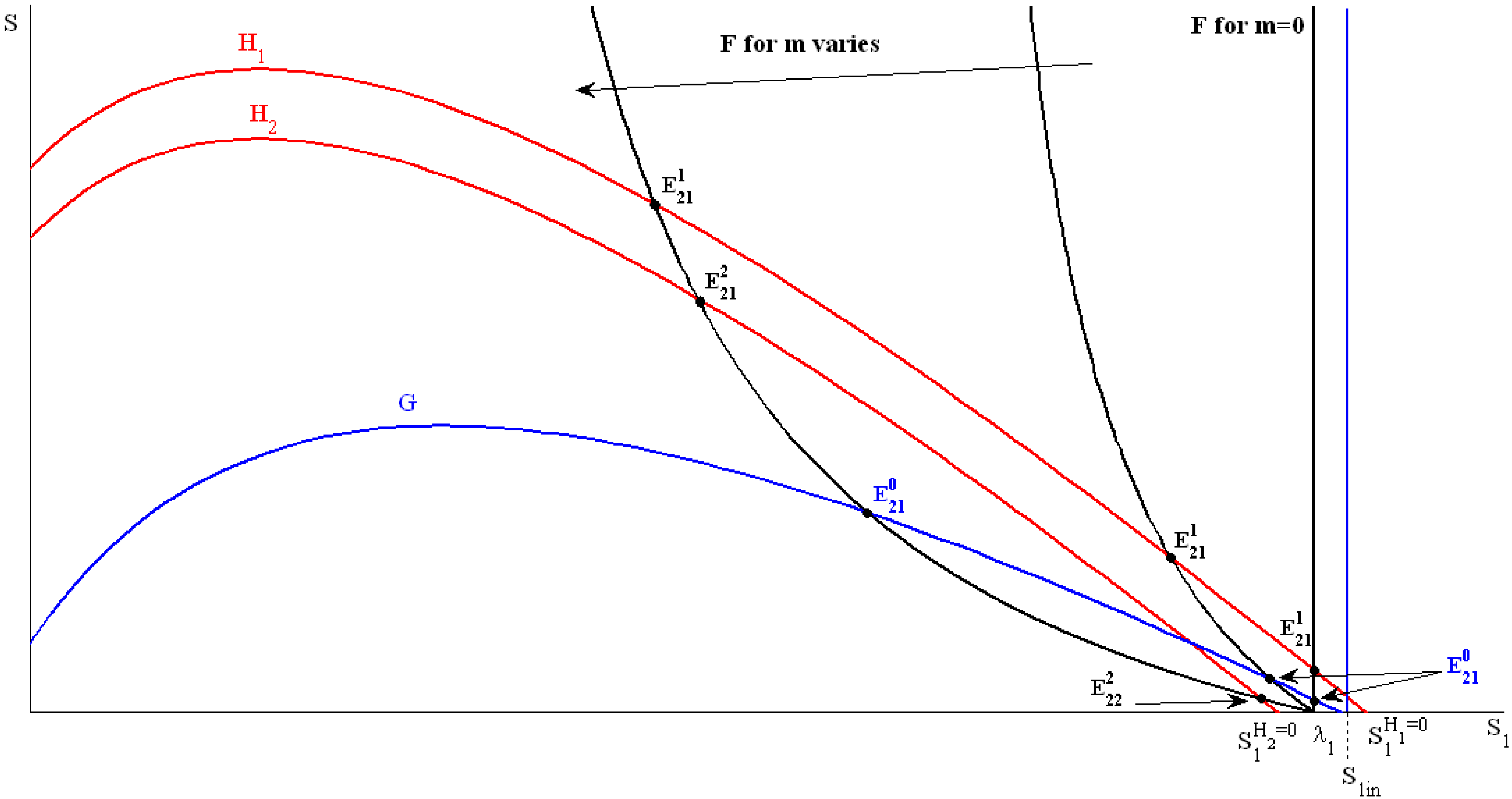
-The AM2 perturbed by the introduction of SMP keeps the number and the nature of its equilibria (only their values change with *m*).

- For the values of *m* close to *1* (sufficiently larger than *0*), we have high concentrations of X_1 and X_2, lower concentrations of S_1, S_2 and S, which is important in this case.

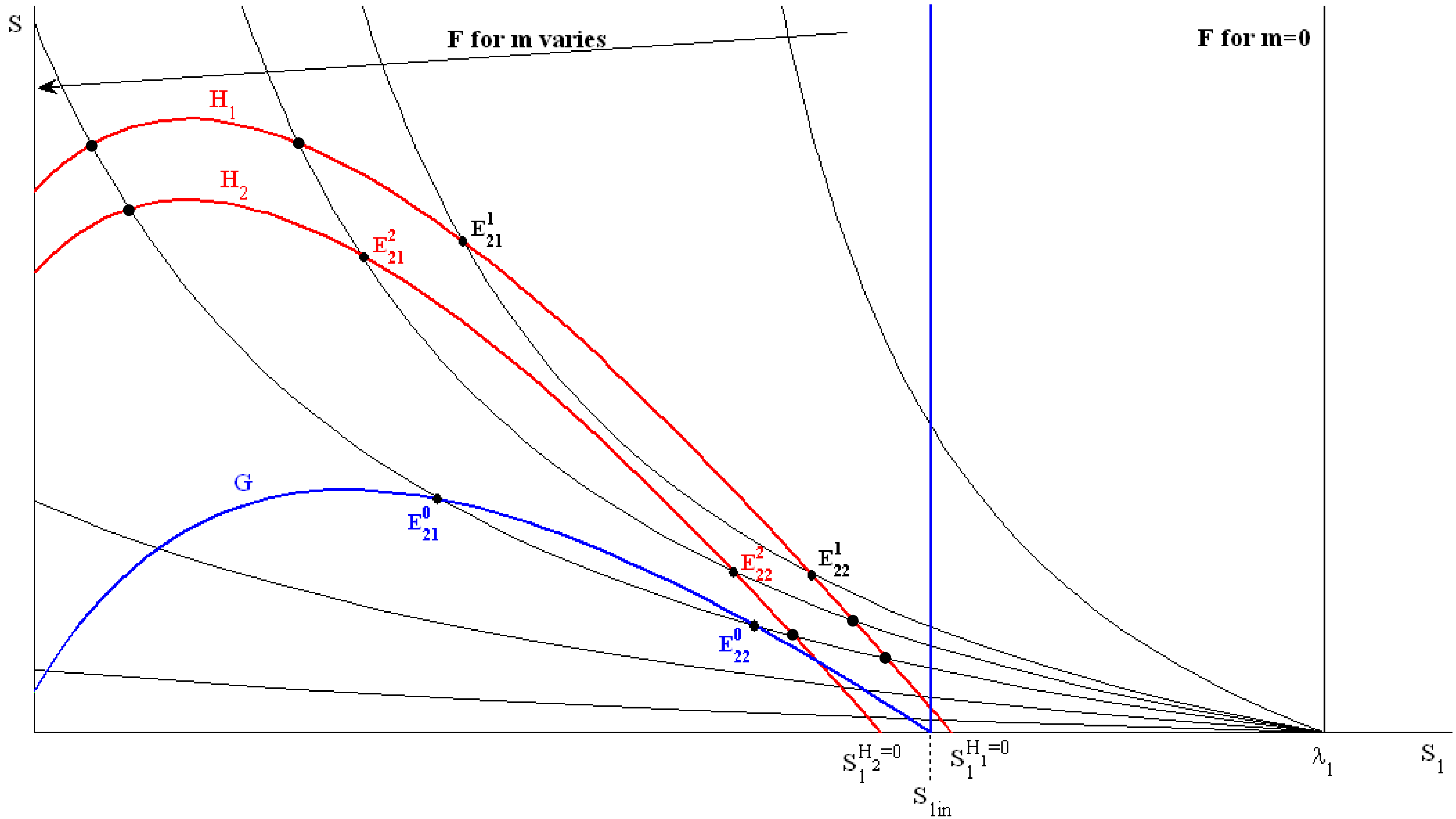
- But, for these values of *m*, the attraction field of the operational equilibrium is restricted, which weakens system stability.

- in this case, it is important from the practical point of view to synthesize control laws stabilizing the system around this operational equilibrium.

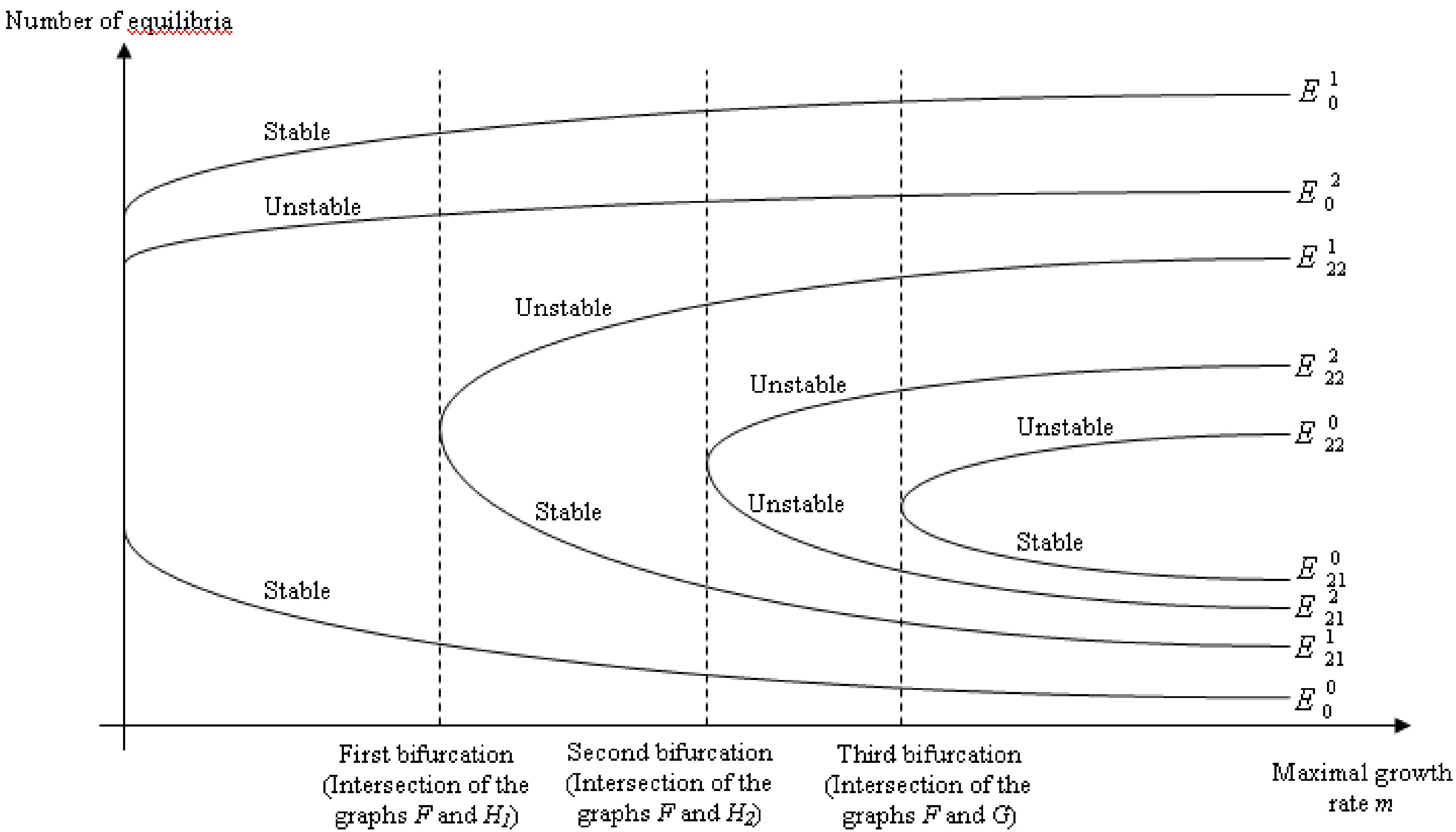
Case 2: $S_1^{H_2=0} < \lambda_1 < S_{1in} < S_1^{H_1=0}$



Case 3: $S_1^{H_2=0} < S_{1in} < S_1^{H_1=0} < \lambda_1$



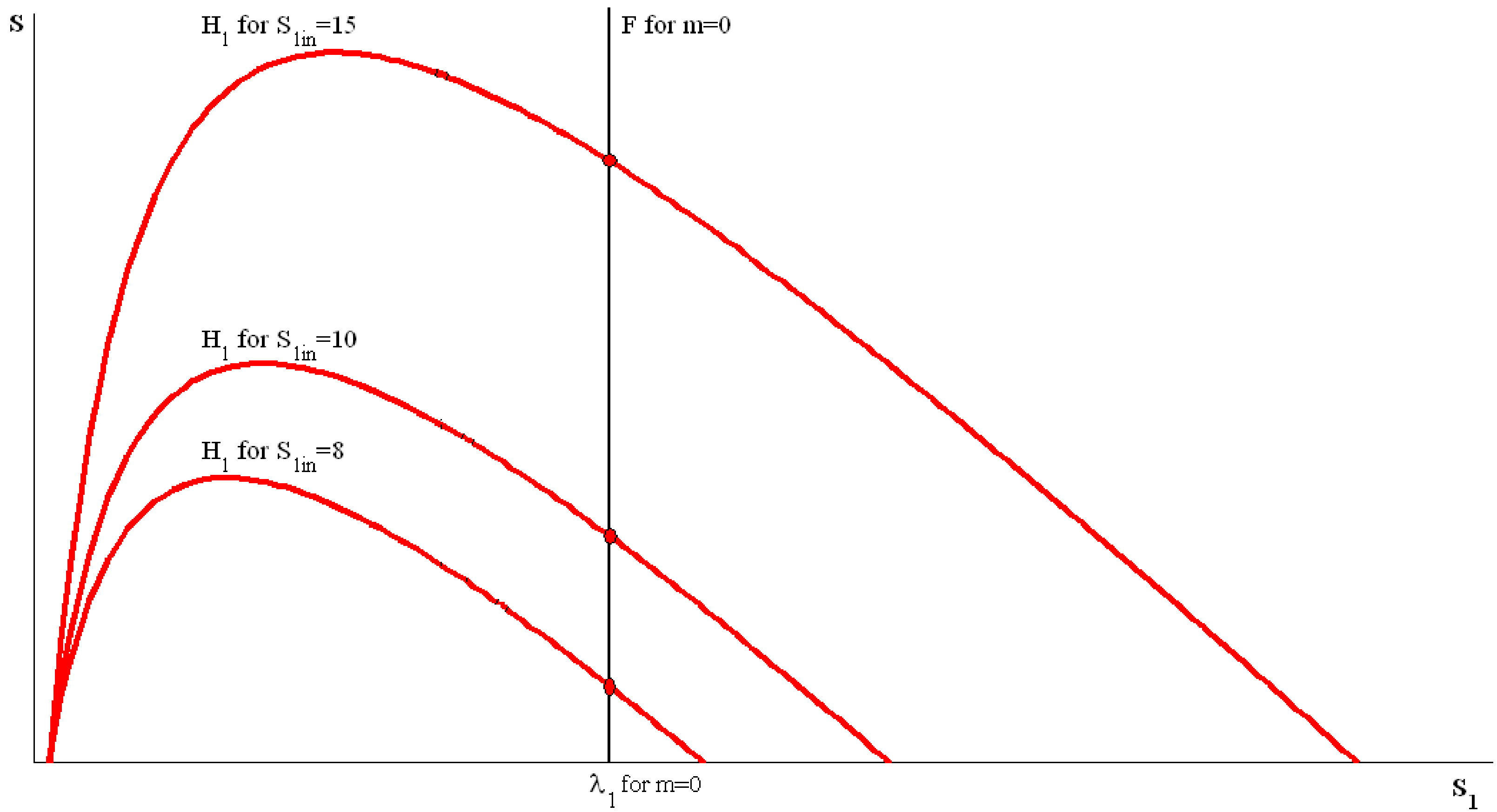
Equilibria bifurcation



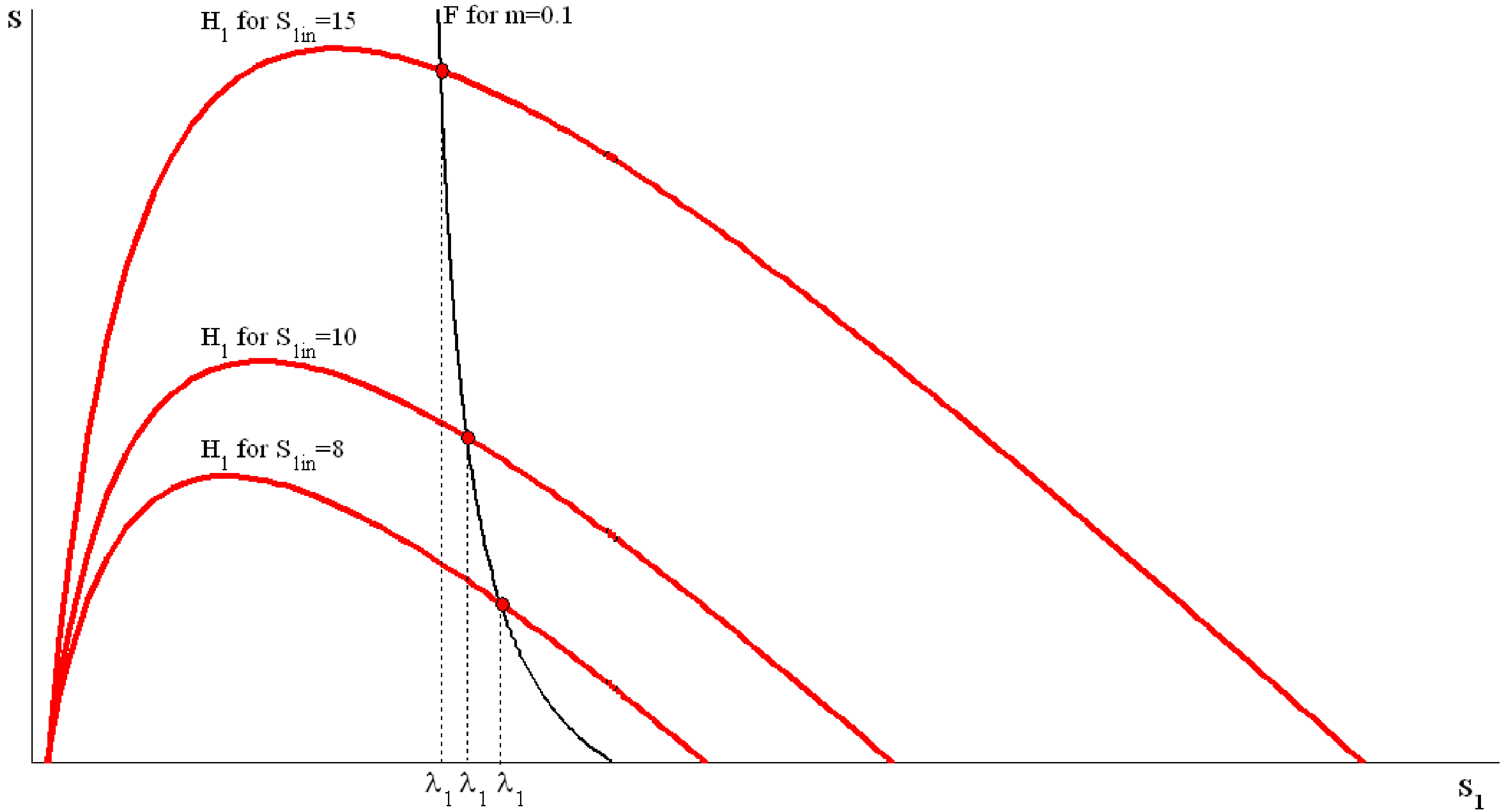
Does SMP integration in the anaerobic digestion models (like AM2) have an interest?

For $m=0$, the AM2b model behaves exactly as the AM2 model.

If S_{1in} changes ➔ λ_1 do not change.



For $m \neq 0$: If S_{1in} increases ➔ λ_1 decreases



Since the equilibrium λ_1 of the AM2b model is calculated by the resolution of the systems:

$$F(S) := \mu_1^{-1}(D_0 + D_1 - \mu(S))$$

Contains explicitly the parameter m in the function $F(S)$.

$$G(S_1) := \frac{1}{B}[S_{1in} - S_1][\frac{1}{k_1}(b_3 + b_1) + \frac{1}{k_1\mu_1}(D_0 - b_1(D_1 + D_0))]$$

$$H_i(S_1) := \frac{1}{B}[A(S_{2in} - \lambda_2^i) + (S_{1in} - S_1)(\frac{A_1 - A_2}{k_1} + \frac{A_2(D_1 + D_0) + D_0}{k_1\mu_1})], \quad i = 1, 2$$

The SMP integration in the model, can predict the change of equilibrium λ_1, which can occur, when the influent concentration S_{1in} of the organic matter changes.

To verify with experimental data for a dilution rate maintained constant for a long time (sufficient steady state) …?

Thank you