Stability Analysis of Some Nonlinear Anaerobic Digestion Models

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Abstract: *The paper deals with local asymptotic stability analysis of some mass balance dynamic models (based on one and on two-stage reaction schemes) of the anaerobic digestion (AD) in CSTR. The equilibrium states for models based on one (with Monod, Contois and Haldane shapes for the specific growth rate) and on two-stage (only with Monod shapes for both the specific growth rate of acidogenic and methanogenic bacterial populations) reaction schemes have been determined solving sets of nonlinear algebraic equations using Maples. Their stability has been analyzed systematically, which provides insight and guidance for AD bioreactors design, operation and control.*

Keywords: *Anaerobic digestion, CSTR, Mathematical modelling, Mass balance non-linear dynamic models, Local stability analysis.*

Introduction

Anaerobic digestion (AD) is an effective biotechnological process for treatment of different agricultural, municipal and industrial wastes [1]. It combines environmental depollution (ecological aspect) with production of renewable energy – biogas, which main component is methane (energetical aspect).

AD is a very unstable process in regard to the biogas reactors (digesters) operation. This is due to the complicated interactions between different microbial species as well as of the complex transformations of the organic matter affected by a variety of environmental factors [1]. In this context use of mathematical models is a powerful tool for investigations, optimization and control of the anaerobic biodegradation [2-8]. More than 750 papers in this field are published during the last 30 years (the half of them – during the last 5 years).

Depending on the aim of the modelling, a large number of modelling approaches are available. From a general point-of-view, they can be classified within three important classes: mass balance models, consisting of sets of non-linear ordinary differential equations (ODE) and describing more accurately all microbiological and biochemical phenomena during the AD processes; black box models (linear or non-linear); heuristic models, based on qualitative and fuzzy logic

The biggest spread for AD processes is received dynamical type of models, based over mass balances and especially such of them, which are created for continuously stirred tank reactor (CSTR) mode.

AD processes have more than one stable stationary solution and the attractive domains of the stable solutions vary with the key parameters. Thus, some initial transient process moving toward one stable solution could suddenly move toward another solution, at which a so-called catastrophe takes places (e.g. washout of microorganisms). That is why it is very important to study the stationary solutions with their associated stability [11, 12]. In [11] local asymptotic stability of the closed loop system (two bacterial populations model with nonlinear output feedback control) is proved decomposing the two populations model into two subsystems. In [12] the stability of the three equilibria and the bifurcation of a modified two populations model of the AD have been analyzed with regard to variations of one and two parameters, using a lot of simplification of the model. Some conclusions (very useful for practice) have been drowning.

The aim of this paper is to present our results concerning the local stability of some AD models.

Mass balance models
Model based on one-stage reaction scheme
Anaerobic digestion is a multistep process involving the action of multiple microbes. Usually, such processes contain a particular step, the so-called rate limiting or rate-determining step, which, being the slowest, limits the rate of the overall process. Lawrence [3] defined as limiting step "that step which will cause process failure to occur under imposed conditions of kinetic stress". The first attempts for modeling anaerobic digestion led to models describing only the limiting step. However, during a wide range of operating conditions, the limiting step is not always the same. It may depend on wastewater characteristics, hydraulic loading, temperature, etc. Andrews [3] for example considered acetogenic methanogenesis as the limiting, O'Rourke [3] – the conversion of fatty acids to biogas, and Eastman and Ferguson [3] – the hydrolysis of biodegradable suspended solids.

It is apparent that the "limiting step hypothesis" leads to simple and readily usable models. Such models, however, do not describe very well the anaerobic bioreactor (digester) behaviour, especially under transient operating conditions [3].

The Graef and Andrews model [2] involves only the acetoclastic methanogens. The conversion of volatile fatty acids into biogas is considered limiting. This is the first and the most simplified model for description of the AD process describing the process rate limiting methanogenic step [4, 7]:

$$\frac{dX}{dt} = \mu X - DX \tag{1}$$

$$\frac{dS}{dt} = -k_1 \mu X + D(S_{0i} - S) \tag{2}$$

$$Q = k_2 \mu X, \tag{3}$$

where S – substrate (acetate) concentration, g·dm^{-3}; X – biomass concentration, g·dm^{-3}; D – dilution rate, day^{-1}; S_{0i} – concentration of inlet organics, g·dm^{-3}; Q – biogas flow rate,

$dm^3 \cdot day^{-1}$; μ – specific growth rate, day^{-1}; k_1 and k_2 are yield coefficients. The specific growth rate (μ) is with one from the following expressions:

– Monod type: $\mu = \dfrac{\mu_{max}S}{\left(k_s + S\right)}$, $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (4)

– Contois type: $\mu = \dfrac{\mu_{max}S}{\left(k_m X + S\right)}$, $\qquad\qquad\qquad\qquad\qquad\qquad\quad$ (5)

– Haldane type: $\mu = \dfrac{\mu_0 S}{\left(k_s + S + S^2 / k_i\right)}$, $\qquad\qquad\qquad\qquad\qquad\quad$ (6)

where μ_{max}, μ_0, k_m, k_s, and k_i are kinetic coefficients.

According to this model, a digester is expected to fail whenever, for some reason, the fatty acid concentration is increased. This causes a drop in the pH and a rise in the acetic acid concentration. This in turn causes a drop in the growth rate of the methanogenic population, until they are washed out, if the situation is prolonged.

It has been proved that this model poses single maximum of the static characteristic $Q = Q(D)$ [7]. This simple nonlinear model is very useful for testing different control algorithms.

Models based on two-stage scheme
Moletta et al. [8] involve an acidogenic step, that forms acetate from glucose, and are inhibited by acetic acid. The overall AD model in this case is as follows:

$$\frac{dX_1}{dt} = \mu_1 X_1 - DX_1$$

$$\frac{dS_1}{dt} = -k_1 \mu_1 X_1 + D\left(S_{0i} - S_1\right)$$

$$\frac{dX_2}{dt} = \mu_2 X_2 - DX_2$$

$$\frac{dS_2}{dt} = -k_2 \mu_2 X_2 + k_3 \mu_1 X_1 - DS_2 \qquad\qquad\qquad (7)$$

$$Q = k_4 \mu_2 X_2,$$

where X_1 and X_2 – concentrations of acidogenic (with specific growth rate μ_1, day^{-1}) and methanogenic (with specific growth rate μ_2, day^{-1}) bacteria, respectively, $g \cdot dm^{-3}$; S_1 – glucose concentration, $g \cdot dm^{-3}$; S_2 – acetate concentration, $g \cdot dm^{-3}$; Q – biogas flow rate, $dm^3 \cdot day^{-1}$; D – dilution rate, day^{-1}; S_{in} – concentration of inlet glucose, $g \cdot dm^{-3}$. In the model (7) k_i ($i = 1 - 4$) – are yield coefficients, μ_1 is with the Monod form (4) and μ_2 – with Haldane form (6); μ_{1max}, μ_{2max}, k_{s1}, k_{s2} and k_{i2} are kinetic coefficients.

It has been proved that this model poses single maximum of the static characteristic $Q = Q(D)$ [9]. This nonlinear model is very useful also for testing different control algorithms.

Local stability analysis

Model based on one stage reaction scheme

Equilibrium points

It is a basic feature of nonlinear systems in general, and consequently of the model (1) – (2) in particular, that the equilibrium states can be stable or unstable depending on the operating point. The equilibrium pointes (for given constant values D^* and S_{0i}) for the model (1) – (3) are well known [4, 7]:

Point 1. The digester is in stationary state when there are no more microorganisms in it, that is when $X = 0$. In this case, it follows from the model (1) – (2) that $D = 0$ or $S = S_{0i}$:

$$\begin{bmatrix} X^* \\ S^* \end{bmatrix} = \begin{bmatrix} 0 \\ S_{0i}^* \end{bmatrix}. \tag{8}$$

This state (8) of the digester will be referred as the *extinguishing equilibrium point*.

Point 2. Depending on values of constant inputs D^* and S_{0i}, there may be steady states for the digester other than the extinguishing equilibrium point. If any, such an equilibrium point will be called *main equilibrium point.* Main equilibrium points are with *nonzero* concentration of microorganisms, and they verify the following equations:

$$\begin{cases} \mu(X^*, S^*) = D^*, \\ X^* = \dfrac{1}{k_1}(S_{0i} - S^*). \end{cases} \tag{9}$$

Monod case

Given the Monod shape (4) for μ (Fig. 1) Eqs. (9) have one, and only one solution if, and only if:

$$D < \mu(S_{0i}^*). \tag{10}$$

So that *for the Monod shape for μ, there is one, and only one equilibrium point (which is then the so-called extinguishing equilibrium point (8)) if and only if :*

$$D \geq \mu(S_{0i}^*), \tag{11}$$

and, there are exactly two equilibrium points (the extinguishing equilibrium point and the main one) if, and only if the condition (10) holds.

Contois case

Given Eqs. (9) the Contois law (5) for μ reads as:

$$\mu(S^*) = \frac{\mu_{max} S^*}{\dfrac{k_m}{k_1} S_{0i}^* + \left(1 - \dfrac{k_m}{k_1}\right) S^*},$$

which reveals μ as an increasing function with respect to S^*.

If $k_m = k_1$ than μ is of the following shape (Fig. 2) and there is one, and only one, so-called main equilibrium point:

$$\begin{bmatrix} X^* \\ S^* \end{bmatrix} = \begin{pmatrix} \dfrac{1}{k_1}\left(1 - \dfrac{D^*}{\mu_{max}}\right)S_{0i}^* \\ \dfrac{D^* S_{0i}^*}{\mu_{max}} \end{pmatrix}$$

provided that $D < \mu_{max}$.

If $k_m < k_1$ than μ is of the following shape (Fig. 3) and again, there is one, and only one, main equilibrium point given by the intersection between the "line D^*" and the curve $\mu(S^*)$ if, and only if, $D \le \mu_{max}$.
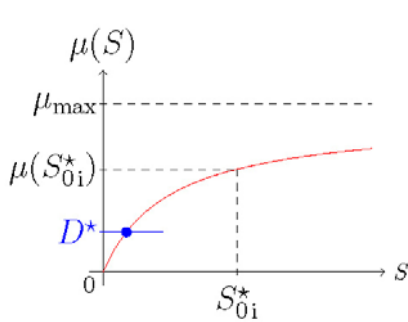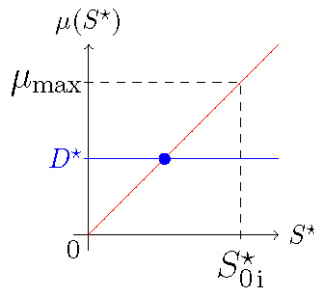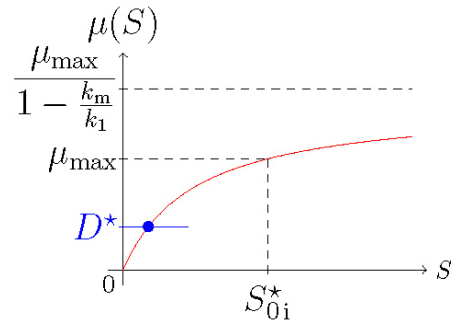

| Fig. 1 | Fig. 2 | Fig. 3 |

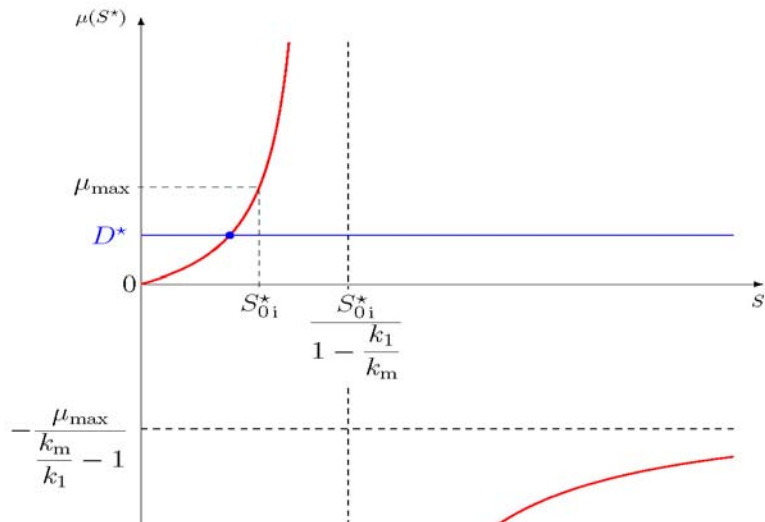If $k_m > k_1$ than μ is of the following shape (Fig. 4):

Fig. 4

and again, there is one, and only one, main equilibrium point given by the intersection between the "line D^*" and the upper part of the curve $\mu(S^*)$ if, and only if, $D \le \mu_{max}$.

Haldane case
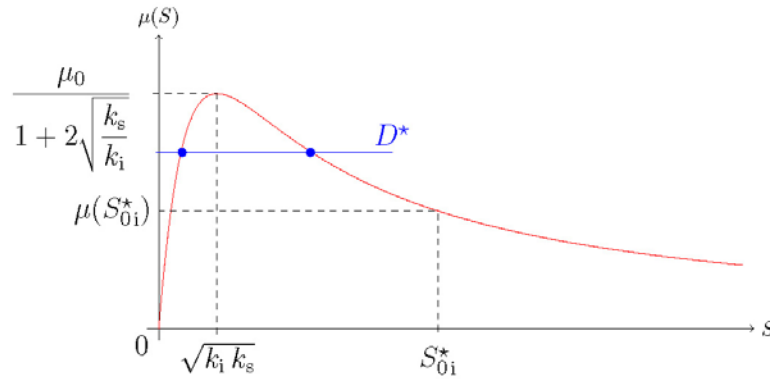Given the Haldane shape (6) for μ (Fig. 5):

Fig. 5

there is one, and only one, main equilibrium point if, and only if:

$$
\begin{cases} D^* \le \mu(S_{0i}^*), \\ S_{0i} \le \sqrt{k_i k_s}, \end{cases} \text{ or } \begin{cases} D^* \le \mu(S_{0i}^*), \\ S_{0i} \ge \sqrt{k_i k_s}, \end{cases} \tag{12}
$$

and there are exactly two main equilibrium points if, and only if:

$$
\begin{cases} \mu(S_{0i}^*) \le D^* < \dfrac{\mu_0}{(1 - 2\sqrt{\dfrac{k_s}{k_i}})}, \\ S_{0i}^* > \sqrt{k_i k_s}. \end{cases} \tag{13}
$$

Stability of the equilibrium points
The analysis of the equilibrium states of the model (1) – (2) will be performed under the following realistic assumptions [4]:

$D(t) \ge 0,\ \forall\ t,\ 0 \le S_{0i} \le S_{\max},\ X(t) \ge 0;\ S(t) \ge 0.$

The Jacobian matrix of the model (1) – (2) at the *extinguishing equilibrium point* is $F(D^*, S_{0i}^*, X^*, S^*)$, where

$$
F(D, S_{0i}, X, S) = \begin{pmatrix} \dfrac{\partial(\mu X - DX)}{\partial X} & \dfrac{\partial(\mu X - DX)}{\partial S} \\ \dfrac{\partial(-k_1 \mu X + D(S_{0i} - S))}{\partial X} & \dfrac{\partial(-k_1 \mu X + D(S_{0i} - S))}{\partial S} \end{pmatrix}.
$$

Therefore

$$
F(D, S_{0i}, X, S) = \begin{pmatrix} \mu(X^*, S^*) - D^* & 0 \\ -k_1 \mu(X^*, S^*) & -D \end{pmatrix},
$$

and *for any for shape of μ the extinguishing equilibrium point is locally asymptotically stable if, and only if:*

$$D > \mu(X^*, S^*). \tag{14}$$

Similarly, the Jacobian matrix of the model (1) – (2) at the main equilibrium point (if any) is $F(D^*, S_{0i}^*, X^*, S^*)$, where

$$F(D, S_{0i}, X, S) = \begin{pmatrix} \dfrac{\partial \mu(X, S)}{\partial X} X & \dfrac{\partial \mu(X, S)}{\partial S} X \\ -k_1 \left(\mu(X, S) + \dfrac{\partial \mu(X, S)}{\partial X} X \right) & -k_1 \dfrac{\partial \mu(X, S)}{\partial S} X - D \end{pmatrix}.$$

The matrix $F(D^*, S_{0i}^*, X^*, S^*)$ is Hurwitz if, and only if, its determinant is positive and its trace negative, that is:

$$\begin{cases} \dfrac{\partial \mu(X^*, S^*)}{\partial S} X^* (D^* + \dfrac{\partial \mu(X^*, S^*)}{\partial X} X^*) - \dfrac{\partial \mu(X^*, S^*)}{\partial X} X^* (k_1 \dfrac{\partial \mu(X^*, S^*)}{\partial S} X^* + D^*) > 0 \\ \dfrac{\partial \mu(X^*, S^*)}{\partial X} X^* - k_1 \dfrac{\partial \mu(X^*, S^*)}{\partial S} X^* - D^* < 0 \end{cases}. \tag{15}$$

The stability of the main equilibrium points is examined through the three empirical laws for the specific growth rate (4), (5) and (6).

Monod case
In this case and under the condition (10) of existence of the unique main equilibrium point, the latter is asymptotically stable if, and only if:

$$\begin{cases} \dfrac{\partial \mu(X^*, S^*)}{\partial S} X^* D^* > 0 \\ -k_1 \dfrac{\partial \mu(X^*, S^*)}{\partial S} X^* - D^* < 0 \end{cases}.$$

These conditions being always satisfied, *there is a main equilibrium point, it is unique and asymptotically stable if, and only if, condition (10) holds.*

Contois case
In this case *the existence, uniqueness and asymptotical stability of the main equilibrium point holds if, and only if $D^* < \mu_{\max}$.*

This results from the fact that:

$$\begin{cases} D^* + \dfrac{\partial \mu(X^*, S^*)}{\partial X} X^* = \dfrac{D^{*2}}{\mu_{\max}} \\[3mm] \dfrac{\partial \mu(X^*, S^*)}{\partial X} X^* = -\dfrac{(\mu_{\max} - D^*)D^*}{\mu_{\max}} \end{cases}$$

and since $\dfrac{\partial \mu(X^*, S^*)}{\partial S}$ is always positive, conditions (15) are easily checked to be verified for all three cases $k_m = k_1$, $k_m < k_1$ and $k_m > k_1$.

Haldane case
In this case and under the condition (12), the main equilibrium point is asymptotically stable. This results from the fact that:

$$\begin{cases} \dfrac{\partial \mu(X^*, S^*)}{\partial X} = 0 \\[3mm] \dfrac{\partial \mu(X^*, S^*)}{\partial S} > 0 \end{cases},$$

so that conditions (15) are easily checked to be verified.

For Haldane law for μ and under the condition (13), the main equilibrium point with positive derivative of μ at X* is asymptotically stable, and the second main equilibrium point is unstable.

This results from the fact that the first condition in (15) is violated when the derivative of μ at X^* is negative.

Model based on two-stage stage reaction scheme
Equilibrium points
In this case there are three equilibrium points:

$$1) \begin{pmatrix} X_1^* \\ S_1^* \\ X_2^* \\ S_2^* \end{pmatrix} = \begin{pmatrix} 0 \\ S_{0i} \\ 0 \\ 0 \end{pmatrix}, \quad 2) \begin{pmatrix} X_1^* \\ S_1^* \\ X_2^* \\ S_2^* \end{pmatrix} = \begin{pmatrix} \dfrac{\mu_1(S_{0i}^*) - D^*}{k_1 \dfrac{\mu_{1\max} - D}{k_{s1} + S_{0i}^*}} \\[4mm] \dfrac{k_{s1} D^*}{\mu_{1\max} - D^*} \\[4mm] 0 \\[4mm] k_3 X_1^* \end{pmatrix}, \quad 3) \begin{pmatrix} X_1^* \\ S_1^* \\ X_2^* \\ S_2^* \end{pmatrix} = \begin{pmatrix} \dfrac{\mu_1(S_{0i}^*) - D^*}{k_1 \dfrac{\mu_{1\max} - D}{k_{s1} + S_{0i}^*}} \\[4mm] \dfrac{k_{s1} D^*}{\mu_{1\max - D^*}} \\[4mm] A \\[4mm] \dfrac{k_{s2} D^*}{\mu_{2\max - D^*}} \end{pmatrix},$$

where the last component of the equilibrium point 2) involves the first component X_1^* of the same equilibrium point 2), and where the quantity A in the equilibrium point 3) is given by the following expression:

$$A = \frac{(k_3 S_{0i}^* + k_3 k_{s1} + k_1 k_{s2})D^{*2}}{k_1 k_2 (\mu_{1\max} - D^*)(\mu_{2\max} - D^*)} -$$

$$- \frac{(k_3 (\mu_{1\max} + \mu_{2\max})S_{0i}^* + k_{s2} k_1 \mu_{1\max} + k_{s1} k_3 \mu_{2\max})D^* + k_3 \mu_{1\max} \mu_{2\max} S_{0i}^*}{k_1 k_2 (\mu_{1\max} - D^*)(\mu_{2\max} - D^*)}.$$

Equilibrium point 1) will be named the *extinguishing equilibrium point* since it corresponds to the situation where there are no more microorganisms (neither acidogenic nor methanogenic) in the anaerobic bioreactor.

Equilibrium point 2) will be named the *methanogenic extinguishing equilibrium point* since it corresponds to the situation where there are no more methanogenic microorganisms while the acidogenic microorganisms are still present in the anaerobic bioreactor. Its first two components are easy seen as the main equilibrium point of the one-stage model, that is, they are the solution of Eqs. (9), where μ is Monod type and S is replaced by S_1. The last two components are the extinguishing equilibrium point of the one-stage model in which $k_3 X_1^*$ (found in the previous first two components) is substituted for S_{0i}.

Equilibrium point 3) will be named the *main equilibrium point of the two-stage model.* Its first two components are the main equilibrium point of the one-stage model, that is, they are the non trivial solution of Eqs. (9) where μ is Monod type and S is replaced by S_1. Its last two components are the main equilibrium point of the one-stage model in which $k_3 X_1^*$ (found in the previous first two components) is substituted for S_{0i}.

Given Eq. (7), and assuming Monod shapes for the specific growth rates μ_1 and μ_2, the Jacobian matrices of the system (7) are all of the form:

$$F(D^*, S_{0i}^*, X^*, S^*) = \begin{pmatrix} F_1(D^*, S_{0i}^*, X^*, S^*) & 0 \\ \\ * & F_2(D^*, S_{0i}^*, X^*, S^*) \end{pmatrix}$$

where

$$F_1(D, S_{0i}, X, S) = \begin{pmatrix} \dfrac{\partial(\mu_1 X_1 - DX_1)}{\partial X_1} & \dfrac{\partial(\mu_1 X_1 - DX_1)}{\partial S_1} \\ \dfrac{\partial(-k_1 \mu_1 X_1 + D(S_{0i} - S_1))}{\partial X_1} & \dfrac{\partial(-k_1 \mu_1 X_1 + D(S_{0i} - S_1))}{\partial S_1} \end{pmatrix}$$

$$F_2(D, S_{0i}, X, S) = \begin{pmatrix} \dfrac{\partial(\mu_2 X_2 - DX_1)}{\partial X_2} & \dfrac{\partial(\mu_2 X_2 - DX_2)}{\partial S_2} \\ \dfrac{\partial(-k_2 \mu_2 X_2 + k_3 \mu_1 X_1 - DS_2)}{\partial X_2} & \dfrac{\partial(-k_2 \mu_2 X_2 k_3 \mu_1 X_1 - DS_2)}{\partial S_2} \end{pmatrix}$$

and * designates a non necessarily zero sub-matrix.

The characteristic polynomial of $F(D^*, S_{0i}^*, X^*, S^*)$ is the product of those of $F_1(D^*, S_{0i}^*, X^*, S^*)$ and $F_2(D^*, S_{0i}^*, X^*, S^*)$.

An equilibrium point is thus asymptotically stable if, and only if, $F_1(D^*, S_{0i}^*, X^*, S^*)$ and $F_2(D^*, S_{0i}^*, X^*, S^*)$ are both Hurwitz. The matrix $F_1(D^*, S_{0i}^*, X^*, S^*)$ is Hurwitz means that the first two components of the equilibrium point form an equilibrium point which is asymptotically stable for the one-stage model where S is replaced by S_1 and X by X_1. And the matrix $F_2(D^*, S_{0i}^*, X^*, S^*)$ is Hurwitz means that the last two components of the same equilibrium point form an equilibrium point which is asymptotically stable for the one-stage model where S is replaced by S_2, X by X_2 and S_{0i} by $k_3 X_1^*$ (found in the previous first two components).

Applying the previous rule it immediately follows that the **extinguishing equilibrium point** is asymptotically stable if, and only if, $F_1(D^*, S_{0i}^*, X^*, S^*)$ and $F_2(D^*, S_{0i}^*, X^*, S^*)$ are Hurwitz when evaluated at this equilibrium point, that is, if and only if:

$$D^* > \mu_{1\max}.$$

By the same rule the **methanogenic extinguishing equilibrium point** is asymptotically stable if, and only if, the corresponding condition (10):

$$D^* < \mu_1(S_{0i}^*),$$

and the corresponding condition (11):

$$D^* > \mu_2(k_3 X_1^*),$$

are satisfied, where X_1^* is as in 2):

$$X_1^* = \frac{\mu_1(S_{0i}^*) - D^*}{k_1 \dfrac{\mu_{1\max} - D}{k_{s1} + S_{0i}^*}}.$$

Put together these two conditions read as:

$$\mu_2\left(k_3 \frac{\mu_1(S_{0i}^*) - D^*)}{k_1 \dfrac{\mu_{1\max} - D^*}{k_{s1} + S_{0i}^*}} \right) < D^* < \mu_1(S_{0i}^*).$$

*The **main equilibrium point** of the two-stage model is asymptotically stable if, and only if, the corresponding condition (10):*

$$D^* < \ \min\left(\mu_1(S_{0i}^*),\, \mu_2\left(k_3\,\frac{\mu_1(S_{0i}^*) - D^*}{k_1\,\dfrac{\mu_{1\max} - D^*}{k_{s1} + S_{0i}^*}}\right)\right)$$

is satisfied.

Conclusions and future work

Different models of the AD of organic wastes have been developed. They can be used for process studies [1, 4], software sensors design [10], and control [6, 9]. In all cases model stability study is very important.

From the above-presented study, concerning local stability analysis of the adopted AD models, the following generalized remarks could be summarized:

1. For one stage AD model (describing the methanogenic stage) with Monod, Contois and Haldane shapes for the specific growth rate, there exists only one asymptotically stable equilibrium point, if and only if, one upper bound for *D* is satisfied.
2. For two stage AD model only with Monod shapes for both specific growth rate of acidogenic and methanogenic bacterial populations, there exists only one asymptotically stable equilibrium point, if and only if, one upper bound for *D* is satisfied.

These remarks may be useful for maximising biogas production from the digester.

In this paper local stability of some AD models has been analyzed using the Lyapunov's first method. Some open problems concerning AD models stability are: steady-state analysis (including local stability) of more complex models and global stability study.

Acknowledgements

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