

Evaluation of Steady State Multiplicity for the Anaerobic Degradation of Solid Organic Waste

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Abstract

This paper evaluates the number and stability of steady states of a two-population model, describing the anaerobic degradation of solid organic waste. Analytical conditions are provided, which define in the input space regions characterized either by a different number or change of stability of steady states. The qualitative results do not depend on the parameter values and allow the proper selection of inputs and initial conditions to achieve a good operation of the process.

Keywords: anaerobic digestion, microbial kinetics, mathematical modelling, nonlinear dynamics

1. Introduction

Anaerobic digestion is a consolidated technology because it has remarkable advantages, such as low energy consumption, less sludge production compared to aerobic processes and direct production of biogas. The total annual potential production of this renewable energy source is estimated at around 200 billions m³ (Appels et al., 2008). One of the most important applications is the biomethanization of organic solid waste, mainly sewage sludge and municipal solid waste.

Several mathematical models have been developed for the anaerobic digestion process. The most well known is Anaerobic Digestion Model no1 described in (Batstone et al., 2002). However, its use in industrial applications is limited, due to the high number of variables and parameters involved, which makes the identification a delicate task. Therefore, simplified models have been developed in order to ease the parameter identification, model validation and design of control strategies. Commonly, the methanogenesis reaction is described as the critical step of the process, even though the hydrolysis reaction (first step of the process) plays also an important role in the anaerobic digestion of solid waste, as it has a limiting effect on the process (Pavlostathis and Giraldo-Gomez, 1991; Batstone et al., 2009).

The steady state behaviour of biological conversion systems (such as the anaerobic digestion process) is an important aspect for the process design and control. Particularly, process conditions under which steady state multiplicity occurs should be accurately identified (Volcke et al., 2010). When the process is characterized by steady state multiplicity, its time evolution is not fully determined by the choice of inputs but also by the initial reactor conditions. This paper evaluates the occurrence of multiple steady states in a two-population model, describing the anaerobic digestion of solid waste. The stability of the physical steady states is assessed. Analytical conditions are provided, which define regions in the input space characterized by a different number of steady states and/or

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change of stability of the steady states. Simulation results are presented to illustrate the importance of initial conditions for the proper operation of the process.

2 Process model

The model, developed by Vavilin and Angelidaki (2005), considers two reactions: hydrolysis and methanogenesis. The biological transformations are described by the following reaction network:



In the first reaction acidogens (ξ_3) transforms the particulate organic matter (ξ_1) into volatile fatty acids (ξ_2). In the second reaction, methanogens (ξ_4) consume the volatile fatty acids (ξ_2) and produce methane. $a, b > 0$ are the stoichiometric coefficients. The two reactions are characterized respectively by Contois and Haldane kinetics:

$$r_1(\xi) = \underbrace{\mu_{m_1} \frac{\xi_1}{K_x \xi_3 + \xi_1} \frac{K_{i_1}}{K_{i_1} + \xi_2}}_{\mu_1(\xi)} \cdot \xi_3 \quad r_2(\xi) = \underbrace{\mu_{m_2} \frac{\xi_2}{K_s + \xi_2} \frac{K_{i_2}}{K_{i_2} + \xi_2}}_{\mu_2(\xi)} \cdot \xi_4 \quad (2)$$

For an ideal continuous stirred tank reactor, the system dynamics described by the reaction network (1) are given by the differential equations (3). The equivalent canonical state representation (4) can be obtained (Bastin and Dochain, 1990) by considering the state transformation: $x_1 = \xi_1 + \xi_3$, $x_2 = \xi_2 - a\xi_3 + b\xi_4$, $x_3 = \xi_3$, $x_4 = \xi_4$, with the positiveness constraints of the original states

$$S_x = \{x \in \mathbb{R}^4, x_1 - x_3 \geq 0, x_2 + ax_3 - bx_4 \geq 0, x_3 \geq 0, x_4 \geq 0\}$$

D represents the dilution rate, while ξ_{in_1} and ξ_{in_2} respectively represent the concentrations of the particulate organic matter and volatile fatty acids in the influent.

$$\begin{aligned} \dot{\xi}_1 &= D(\xi_{in_1} - \xi_1) - r_1(\xi) & \dot{x}_1 &= D(\xi_{in_1} - x_1) \\ \dot{\xi}_2 &= D(\xi_{in_2} - \xi_2) + ar_1(\xi) - br_2(\xi) & \dot{x}_2 &= D(\xi_{in_2} - x_2) \\ \dot{\xi}_3 &= -D\xi_3 + r_1(\xi) & \dot{x}_3 &= -Dx_3 + r_1(\xi) \\ \dot{\xi}_4 &= -D\xi_4 + r_2(\xi) & \dot{x}_4 &= -Dx_4 + r_2(\xi) \end{aligned} \quad (3) \quad (4)$$

All steady states lie on the plane $\Delta = \{x \in \mathbb{R}^4, x_1 = \xi_{in_1}, x_2 = \xi_{in_2}\}$ (Sbarciog et al., 2010).

3 Calculation of steady states

The steady states are calculated from (4), by setting the derivative equal to zero. Consequently, the conditions defining S_x are checked to decide whether or not the steady state is physical. All steady states satisfy $x_1 = \xi_{in_1}$, $x_2 = \xi_{in_2}$, $(-D + \mu_1(\xi)) \cdot x_3 = 0$, $(-D + \mu_2(\xi)) \cdot x_4 = 0$. The last two expressions lead to several possibilities, which are briefly discussed below. A capital letter is assigned to each steady state. The analytical expressions of all steady states and the conditions under which they are physical are listed in Table 1.

1. $x_3 = 0, x_4 = 0$: this generates the steady state denoted by A , which represents the total wash out state of the system;
2. $x_4 = 0, \mu_1(\xi) = D$: this generates the steady state denoted by B , which is characterized by the wash out of methanogens. $\xi_{3,B}$ is the unique positive solution of $\mu_1(\xi) = D$, which can be rewritten as a 2nd order equation in ξ_3 ;
3. $x_3 = 0, \mu_2(\xi) = D$: this possibility leads to two steady states denoted by C and D , characterized by the wash out of acidogens. $\xi_{2,C} < \xi_{2,D}$ are the two solutions of $\mu_2(\xi) = D$, which can be rewritten as a 2nd order equation in ξ_2 ;
4. $\mu_1(\xi) = D, \mu_2(\xi) = D$: two steady states E and F are obtained. $\xi_{2,E} < \xi_{2,F}$ are the two solutions of $\mu_2(\xi) = D$, while $\xi_{3,E}$ and $\xi_{3,F}$ are respectively the solutions of $\mu_1(\xi) = D$ for $\xi_2 = \xi_{2,E}$ and for $\xi_2 = \xi_{2,F}$. These steady states correspond to the coexistence of the two species, a situation arising from a syntrophic relationship (methanogens consume the volatile fatty acids which are inhibitory for themselves and in less degree for acidogens).

Steady state	Condition of occurrence
$x_A = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & 0 & 0 \end{bmatrix}^T$ $\xi_A = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & 0 & 0 \end{bmatrix}^T$	N/A
$x_B = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & \xi_{3,B} & 0 \end{bmatrix}^T$ $\xi_B = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & \xi_{3,B} & 0 \end{bmatrix}^T$	$D \leq \mu_{m_1} K_{i_1} / (K_{i_1} + \xi_{in_2})$
$x_C = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & 0 & (\xi_{in_2} - \xi_{2,C})/b \end{bmatrix}^T$ $\xi_C = \begin{bmatrix} \xi_{in_1} & \xi_{2,C} & 0 & (\xi_{in_2} - \xi_{2,C})/b \end{bmatrix}^T$	$D \leq \max(\mu_2(\xi))$ $\xi_{2,C} \leq \xi_{in_2}$
$x_D = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & 0 & (\xi_{in_2} - \xi_{2,D})/b \end{bmatrix}^T$ $\xi_D = \begin{bmatrix} \xi_{in_1} & \xi_{2,D} & 0 & (\xi_{in_2} - \xi_{2,D})/b \end{bmatrix}^T$	$D \leq \max(\mu_2(\xi))$ $\xi_{2,D} \leq \xi_{in_2}$
$x_E = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & \xi_{3,E} & (\xi_{in_2} - \xi_{2,E} + a\xi_{3,E})/b \end{bmatrix}^T$ $\xi_E = \begin{bmatrix} \xi_{in_1} - \xi_{3,E} & \xi_{2,E} & \xi_{3,E} & (\xi_{in_2} - \xi_{2,E} + a\xi_{3,E})/b \end{bmatrix}^T$	$D \leq \max(\mu_2(\xi))$ $D \leq \mu_{m_1} K_{i_1} / (K_{i_1} + \xi_{in_2})$ $\xi_{2,E} - a\xi_{3,E} \leq \xi_{in_2}$
$x_F = \begin{bmatrix} \xi_{in_1} & \xi_{in_2} & \xi_{3,F} & (\xi_{in_2} - \xi_{2,F} + a\xi_{3,F})/b \end{bmatrix}^T$ $\xi_F = \begin{bmatrix} \xi_{in_1} - \xi_{3,F} & \xi_{2,F} & \xi_{3,F} & (\xi_{in_2} - \xi_{2,F} + a\xi_{3,F})/b \end{bmatrix}^T$	$D \leq \max(\mu_2(\xi))$ $D \leq \mu_{m_1} K_{i_1} / (K_{i_1} + \xi_{in_2})$ $\xi_{2,F} - a\xi_{3,F} \leq \xi_{in_2}$

Table 1: Analytical expressions and conditions for the occurrence of steady states

Table 1 shows that, except for the total wash out state, which is independent of the input values, one or more conditions must be satisfied for a steady state to be physical. These conditions are graphically illustrated in Fig. 1 by continuous lines. They define in the space $\xi_{in_2} - D$ various regions, characterized either by a different number or type of steady states. The correspondence is given in Table 2. Note that only the last condition for x_E , respectively x_F , involves ξ_{in_1} . As an example, and in order to obtain a clear representation of the various regions, this condition has been evaluated for a specific value of ξ_{in_1} rather than an interval, and led to the curve separating regions 3 and 5 from regions 2, 4 and 6. This implies that the size of these regions will change depending on the value of ξ_{in_1} .

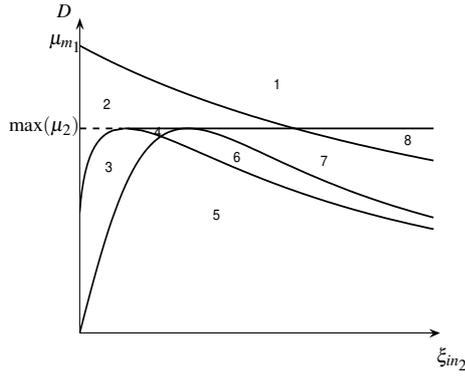


Figure 1: Regions corresponding to the occurrence of various steady states

Region	Physical steady states
1	x_A
2	x_A, x_B
3	x_A, x_B, x_E
4	x_A, x_B, x_E, x_F
5	x_A, x_B, x_C, x_E
6	x_A, x_B, x_C, x_E, x_F
7	$x_A, x_B, x_C, x_D, x_E, x_F$
8	x_A, x_C, x_D

Table 2: Correspondence between the regions and the physical steady states

4 Stability of steady states

The stability of the steady states is assessed using the linearization principle. The Jacobian matrix on the plane Δ is computed and the two eigenvalues are evaluated at each steady state. A steady state is (locally asymptotically) stable if both eigenvalues have negative real parts, and unstable if at least one eigenvalue has positive real part. The index of the steady state is the number of eigenvalues with positive real part. Hence, x_A is stable in regions 1 and 8, has index 1 in 2, 3, 4, 7, and index 2 in regions 5 and 6; x_B is stable in regions 2, 4, 6, 7, and has index 1 in regions 3 and 5; x_C is stable in region 8 and has index 1 in regions 5, 6, 7; x_D is always unstable, either with index 1 in region 8 or index 2 in region 7; x_E is always stable and x_F has always index 1 in the regions where they occur as physical steady states.

5 Discussion

A good operation of a continuous anaerobic digestion system aims at reaching a steady state characterized by the consumption of both particulate organic matter and volatile fatty acids, which is possible only if both type of bacteria are present in the reactor. There are two steady states, which fulfill this condition, x_E and x_F . However only x_E is stable and will be reached in open loop. If ξ_{in1} and ξ_{in2} are such that (ξ_{in2}, D) is in region 3 or 5, then any initial condition characterized by the presence of both populations will lead the process to x_E . On the contrary, if (ξ_{in2}, D) is in region 4, 6 or 7, then some initial conditions will lead the system to x_E , while the rest will determine the convergence to x_B , characterized by the wash out of methanogens and consequently by the accumulation of volatile fatty acids (see Fig. 2). The two sets of initial conditions are separated by the stability boundary of x_E (illustrated by a dashed line in Fig. 2), which can be estimated as described by Sbarciog et al. (2008). Fig. 2 shows the phase portrait of the system on the plane Δ for $\xi_{in1} = 25$ g/L, $\xi_{in2} = 0.02$ g/L and $D = 0.85$ d⁻¹, which correspond to region 4. The numerical values for the system parameters are given in Table 3.

6 Conclusions

In this paper the occurrence of multiple steady states in a two-population model, describing the anaerobic digestion of solid waste, has been evaluated. Analytical conditions have

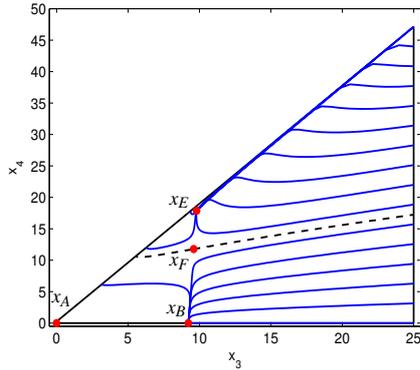


Figure 2: The phase portrait of the system on the plane Δ for choice of inputs in region 4

μ_{m1}	6.8 d^{-1}	μ_{m2}	1.19 d^{-1}
K_x	10.8 g/L	K_s	0.021 g/L
K_{i1}	15 g/L	K_{i2}	1.5 g/L
a	0.15	b	0.08
ξ_{in1}	$[0, 30] \text{ g/L}$	ξ_{in2}	$[0, 5] \text{ g/L}$
D	$[0, 5] \text{ d}^{-1}$		

Table 3: Numerical values of model parameters and inputs

been provided, which define regions in the input space characterized by a different number and/or change of stability of the steady states. The qualitative results do not depend on the parameter values. When steady state multiplicity occurs, the time evolution of the system is not fully determined by the choice of inputs but also by the initial reactor conditions, which should be carefully selected for the good operation of the process.

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