This is an Author's Accepted Manuscript of an article published in Mathematical and Computer Modelling of Dynamical Systems, January 2014, available on-line: http://www.tandfonline.com/doi/full/10.1080/13873954.2013.817443\#.U2D-cfmSyAU

Start-up of Multispecies Anaerobic Digestion Systems: Extrapolation of the Single Species Approach

M. Sbarciog[a**] and A. Vande Wouwer[a]

[a] University of Mons (UMONS), Automatic Control Laboratory,

31 Boulevard Dolez, 7000 Mons, Belgium

Abstract

This paper presents a brief evaluation of a start-up strategy for multispecies anaerobic digestion systems modelled as two-step reaction systems, in which acidogenesis is described by Monod kinetics while the methanogenesis is described by Haldane kinetics. The start-up policy has been developed originally for single species systems with the aim of maximizing the biogas outflow rate. It consists of switching the dilution rate from minimum to maximum and then to the optimal value in order to bring the system from an arbitrary initial condition to the optimal setpoint. This start-up strategy is applied to the multispecies system using an averaged model, which is usually the only model that can be identified for a multispecies system, as measuring individual biomasses is almost impossible in practice. Even the development of an accurate averaged model, fully characterizing the system dynamics based on the variation of the species proportions is difficult. The averaged models used in this study are built based on a more or less accurate knowledge of the species proportions and their kinetics at the start-up instant and used as such in the application of the start-up policy. It is shown that the start-up policy leads to an efficient ecosystem, characterized by high outflow rate of biogas, which is very close to the maximum even in the case of an inaccurate averaged model. The influence of the model accuracy on the system stability and its productivity is discussed. This study can also be viewed as a robustness evaluation with respect to model inaccuracy of the single species start-up strategy, as the process changes from the averaged kinetics to the kinetics of the winning species during species selection.

Keywords— biotechnology, waste treatment, nonlinear systems, optimality, bang-bang control

**Corresponding author. Email: MihaelaIuliana.Sbarciog@umons.ac.be

1 Introduction

Anaerobic digestion is one of the most popular process for the biological treatment of waste or wastewater. It consists of a chain of biological reactions performed by several groups of microorganisms in an oxygen-free environment, in which the influent organic matter is transformed into anaerobic biomass and biogas (mainly methane and carbon dioxide). Compared to the aerobic treatment, the anaerobic digestion provides several advantages among which the higher energy production and the substantially lower sludge production are the most important ones. In terms of process stability, anaerobic digestion still lags behind aerobic biological treatment or physico-chemical processes. Substantial expertise is required to operate such a process properly, as the operational point is not globally stable. Thus a good understanding of process dynamics and an efficient start-up strategy are required to safely drive the reactor towards an optimal operating point.

Many models for anaerobic digestion exist, the most popular for system analysis and process control being the two-step reaction models. Commonly, the models assume that only one species perform the transformation, while in reality the conversion is carried out by a consortium of microorganisms, several hundreds of bacterial and archaeal species [1]. Hence, these models approximate the real system by averaging the dynamics of the species present in the reactor. Reactor start-up is a delicate problem, as not only it has to bring the system to an operational point but it has to lead to a consolidated ecosystem in terms of treatment efficiency and maximization of biogas production. Numerous studies regarding competition between species exist, but not many start-up strategies for multispecies anaerobic digestion systems have been developed. Recently, [2] presented a selective start-up strategy, which drives the competition by regulating the volatile fatty acids concentration. The aim is to select the species with good performance in the standard operating mode of the process.

This paper evaluates the applicability and efficiency of a start-up strategy for the optimization of methane production in a multispecies anaerobic digestion system. This strategy has been developed for a single species model of the system [3, 4]. The central element influencing the stability and the productivity of the multispecies system is the accuracy of the model used for the implementation of the start-up procedure. Two situations are illustrated: i) the case where an initially accurate averaged model based on the exact knowledge of the initial ($t = 0$) species proportions and their kinetics is available (this case will be referred later on as the ”accurate” averaged model); ii) the case where the model does not describe accurately the multispecies system at the initial time. The start-up policy consists of switching the dilution rate between three levels to bring the system to a steady state characterized by a high outflow rate of biogas. The levels of the dilution rate and the instants for switching between them are computed using the system model. On the one hand, the start-up strategy appears as a simple mean to build an efficient ecosystem by driving the competition between the species to select the ones able to enhance system productivity; on the other hand, this study may be seen as a robustness evaluation of the start-up strategy: as the selection process goes on, the system dynamics are better characterized by the kinetics of the favored species rather than the accurate/inaccurate averaged (at the initial time) kinetics.

This paper is organized as follows. The next section introduces the system models, whereas section 3 briefly summarizes the optimization strategy. In section 4, simulation results are thoroughly discussed. Finally, section 5 draws conclusions and suggests research perspectives.

2 The system models

Anaerobic digestion systems are usually modelled as two-step reaction systems [5] for analysis and control purposes, where the considered reactions are acidogenesis and methanogenesis. During acidogenesis, the organic matter ξ_1 is consumed by the acidogenic biomass ξ_3 and volatile fatty acids ξ_2 are produced. During methanogenesis, volatile fatty acids ξ_2 are consumed by the methanogenic biomass ξ_4 and biogas is produced. The acidogenic reaction is limited by the amount of organic matter ξ_1, i.e., the growth of the acidogenic biomass is activated by higher amounts of organic matter (with a saturation at large cocentrations as described by Monod model). The methanogenic reaction is limited by low amounts of volatile fatty acids and inhibited by high amounts of ξ_2, as described by Haldane kinetics.

We study the case when the anaerobic digestion process is operated in continuous mode, i.e., a flow containing organic matter ξ_{in_1} and volatile fatty acids ξ_{in_2} is continuously supplied to the reactor while an equal flow is continuously withdrawn to ensure a constant volume. Assuming that n acidogenic species and m methanogenic species are present in the reactor, whose concentrations are respectively denoted by ξ_3^i (with $i = 1 \dots n$) and ξ_4^j (with $j = 1 \dots m$), a mass balance on the chemostat system leads to the mathematical model:

$$\dot{\xi}_1 = u(\xi_{\text{in}_1} - \xi_1) - a \sum_{i=1}^{n} r_1^i(\xi) \tag{1}$$

$$\dot{\xi}_2 = u(\xi_{\text{in}_2} - \xi_2) + c \sum_{i=1}^{n} r_1^i(\xi) - d \sum_{j=1}^{m} r_2^j(\xi) \tag{2}$$

$$\dot{\xi}_3^i = -u\xi_3^i + r_1^i(\xi) \qquad i = 1 \dots n \tag{3}$$

$$\dot{\xi}_4^j = -u\xi_4^j + r_2^j(\xi) \qquad j = 1 \dots m \tag{4}$$

where u denotes the dilution rate defined as the flow entering the reactor scaled by the reactor volume. The reaction rates

$$r_1^i(\xi) = \mu_1^i(\xi_1)\xi_3^i \qquad r_2^j(\xi) = \mu_2^j(\xi_2)\xi_4^j \tag{5}$$

are characterized respectively by the Monod and Haldane growth functions

$$\mu_1^i(\xi_1) = \mu_{m_1}^i \frac{\xi_1}{K_{s_1}^i + \xi_1} \qquad i = 1 \dots n \tag{6}$$

$$\mu_2^j(\xi_2) = \mu_{m_2}^j \frac{\xi_2}{K_{s_2}^j + \xi_2 + \dfrac{\xi_2^2}{K_{i_2}^j}} \qquad j = 1 \dots m \tag{7}$$

where $K_{s_1}^i$, $K_{s_2}^j$ are half-saturation constants and $K_{i_2}^j$ are inhibition constants. The outflow rate of produced methane gas is given by:

$$Q(\xi) = q \sum_{j=1}^{m} \mu_2^j(\xi_2)\xi_4^j \tag{8}$$

$a, c, d > 0$ are the stoichiometric coefficients and $q > 0$ is the yield for the methane production. The numerical values of the model parameters used in the following simulation studies are taken from [5], where they have been identified from experiments on a real anaerobic digestion system treating vinasses. As the work described in this reference assumes a single species model, values for the kinetic parameters of the other species considered in our study have been arbitrarily selected with a maximum $\pm 50\%$ deviation around the identified values.

An averaged model of the system (1)-(4) can be obtained by lumping the n types of acidogens into one acidogenic species and the m types of methanogens into one methanogenic species, with the growth functions

$$\mu_1^a(\xi_1) = \mu_{m_1}^a \frac{\xi_1}{K_{s_1}^a + \xi_1} \tag{9}$$

$$\mu_2^a(\xi_2) = \mu_{m_2}^a \frac{\xi_2}{K_{s_2}^a + \xi_2 + \dfrac{\xi_2^2}{K_{i_2}^a}} \tag{10}$$

Then, the averaged model becomes

$$\dot{\xi}_1 = u(\xi_{\text{in}_1} - \xi_1) - a\mu_1^a(\xi_1)\xi_3^a \tag{11}$$

$$\dot{\xi}_2 = u(\xi_{\text{in}_2} - \xi_2) + c\mu_1^a(\xi_1)\xi_3^a - d\mu_2^a(\xi_2)\xi_4^a \tag{12}$$

$$\dot{\xi}_3^a = -u\xi_3^a + \mu_1^a(\xi_1)\xi_3^a \tag{13}$$

$$\dot{\xi}_4^a = -u\xi_4^a + \mu_2^a(\xi_2)\xi_4^a \tag{14}$$

and the outflow rate of methane gas reads:

$$Q^a(\xi) = q\mu_2^a(\xi_2)\xi_4^a \tag{15}$$

Necessary conditions for the equivalence between the multispecies model (1)-(4) and the averaged model (11)-(14) are given by the following relationships:

$$\xi_3^a = \sum_{i=1}^{n} \xi_3^i, \qquad \xi_4^a = \sum_{j=1}^{m} \xi_4^j \tag{16}$$

$$\mu_1^a(\xi_1) \cdot \xi_3^a = \sum_{i=1}^{n} \mu_1^i(\xi_1) \cdot \xi_3^i \tag{17}$$

$$\mu_2^a(\xi_2) \cdot \xi_4^a = \sum_{j=1}^{m} \mu_2^j(\xi_2) \cdot \xi_4^j \tag{18}$$

Denoting by $p_{a_i}(t) = \xi_3^i(t)/\xi_3^a(t)$ the proportion of the acidogenic species ($i = 1 \dots n$) and by $p_{m_j}(t) = \xi_4^j(t)/\xi_4^a(t)$ the proportion of the methanogenic species ($j = 1 \dots m$), with

$$\sum_{i=1}^{n} p_{a_i}(t) = 1, \qquad \sum_{j=1}^{m} p_{m_j}(t) = 1 \tag{19}$$

then (17), (18) become

$$\mu_1^a(\xi_1) = \sum_{i=1}^{n} p_{a_i}(t) \cdot \mu_1^i(\xi_1) \tag{20}$$

$$\mu_2^a(\xi_2) = \sum_{j=1}^{m} p_{m_j}(t) \cdot \mu_2^j(\xi_2) \tag{21}$$

Note that the averaged kinetics (20), (21) are time dependent, as species proportions are changing as time evolves. However, since the bacterial proportions cannot be easily measured in practice, further on we denote by ”averaged model” the kinetic parameters identified at the initial time ($t = 0$) based on the exact or approximate knowledge of the species proportions. Hence the averaged models in this paper are models in which the growth functions have constant kinetic parameters.

2.1 Steady state analysis of the averaged model

A detailed analysis of the single species model such as the one characterized by the averaged model dynamics can be found in [6], where it is shown that every system trajectory converges to a steady state lying on the plane

$$\Delta^a = \left\{ \xi^a \in \mathbb{R}^4_+;\ \xi_1 + a\xi_3^a = \xi_{\text{in}_1};\ \xi_2 - c\xi_3^a + d\xi_4^a = \xi_{\text{in}_2} \right\}$$

Depending on the magnitude of the dilution rate u and of the substrate concentrations in the influent ξ_{in_1}, ξ_{in_2}, the averaged model can possess up to six steady states, which can be roughly grouped in wash-out equilibria (characterized by the wash-out of either one or both microorganism types) and operational equilibria (characterized by the presence of both microorganism types). The analytical expressions and the stability properties of all equilibria can be found in [6].

2.2 Steady state analysis of the multispecies model

According to the competitive exclusion principle (CEP), first introduced in [7], at most one of the acidogenic species and one methanogenic species will survive [8]. The winning acidogenic species is the one requiring the smallest amount of nutrient in steady state, while the winning methanogenic species may depend on the initial state of the system [9]. This implies that the multispecies system has the same types of equilibria as the averaged model (or the single species system), all lying in the set

$$\Delta = \left\{ \xi \in \mathbb{R}^{2+n+m}_+;\ \xi_1 + a\sum_{i=1}^{n} \xi_3^i = \xi_{\text{in}_1},\ \xi_2 - c\sum_{i=1}^{n} \xi_3^i + d\sum_{j=1}^{m} \xi_4^j = \xi_{\text{in}_2} \right\}$$

Their analytical expressions are similar to the ones of the single species model, where the concentrations of acidogenic and methanogenic bacteria are respectively replaced by vectors of the form

$$\begin{bmatrix} 0 & \dots & \xi_3^i & \dots & 0 \end{bmatrix}^T \in \mathbb{R}^n_+, \quad \begin{bmatrix} 0 & \dots & \xi_4^j & \dots & 0 \end{bmatrix}^T \in \mathbb{R}^m_+.$$

$i \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$ indicate respectively the winning species.

3 Optimizing control

An important aspect in controlling anaerobic digestion systems is represented by the maximization of biogas production while minimizing or controlling at specified low values the organic load in the effluent. Increasing biogas production implies by default decreasing the organic load in the effluent. However, only the regulation of the organic matter content in the effluent at low values does not necessarily ensure high biogas production on a long term. In this view, a control strategy for maximizing the biogas production in single species anaerobic digestion systems has been presented in [3, 4]. The strategy is based on the system properties and successfully approximates the solution of a classical optimal-control problem for maximizing biogas production during the transient. The transient optimization is coupled with a steady state optimization, which allows to reach the equilibrium characterized by maximum biogas outflow rate.

The strategy proposes to drive the system from an arbitrary initial condition to the optimal steady state by operating the system as follows:

- minimum dilution rate (u_{min}) until the switching surface is reached (the switching surface is the surface in state space which separates a region of minimum control effort from one of maximum control effort);

- maximum dilution rate (u_{max}) until the target set is reached (the target set is the set of desired system states, i.e. the states in this set fulfill some well-defined conditions);

- optimal dilution rate (u_s); then the system settles down in the optimal steady state.

Minimum and maximum dilution rates and the target set are chosen based on the model characteristics, while the optimal dilution rate is the solution of a steady state optimization problem. One of the system stability boundaries is selected as switching surface, which can be accurately estimated using an algorithm such as described in [10, 11]. The selected switching surface separates the region of system states which lead to a methanogens wash-out condition from the region of system states which determine the convergence to a nominal operating point (both acidogens and methanogens are present in the reactor), when the system is operated with the maximum dilution rate u_{max}. This implies that changing the dilution rate from the minimum to the maximum level before the system state reaches the switching surface will cause the wash-out of methanogens. To detect whether or not the switching surface has been reached, measurements of the biomasses and the substrates are required. Further on, it is assumed that the substrate concentrations in the influent are constant and known.

In this work, we apply the optimizing control strategy to the multispecies system (1)-(4) by determining the required key elements using an averaged model of the form (11)-(14). Details regarding the selection of u_{min}, u_{max}, the definition of the target set S and the calculation of u_s can be found in [4]. Here, we evaluate to which extent this start-up procedure leads to a consolidated ecosystem in terms of biogas production maximization and what is the influence of the averaged model accuracy on the stability and efficiency of the process.

4 Simulation results

To evaluate the optimizing control strategy for the multispecies system, we consider further, without loss of generality, that three acidogenic species ($n = 3$) and three methanogenic species ($m = 3$) are present in the reactor at start-up.

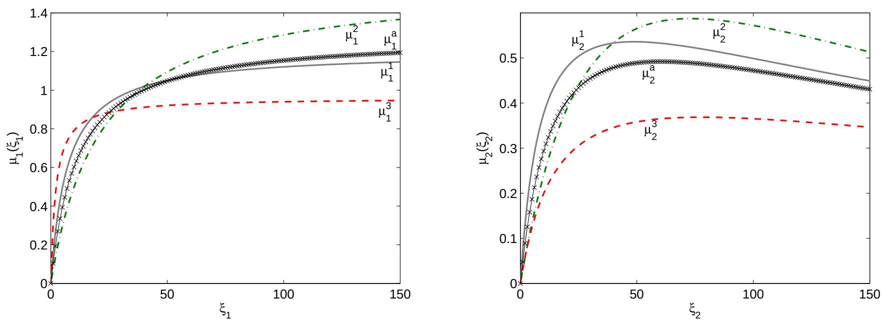
4.1 Accurate averaged model

Numerical values for the kinetic parameters of each species have been generated from the ones used in [4]. They are given in Table 1. Subsequently, an averaged model is identified for the multispecies system, where the parameters of the growth functions $\mu_1^a(\xi_1)$ and $\mu_2^a(\xi_2)$ are found from (20) and (21) using a nonlinear least-squares data-fitting algorithm. The following values have been assumed for the proportions of the species for both model identification and initialization of the simulation: $p_{a_1}(0) = 0.2$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.3$, $p_{m_1}(0) = 0.5$, $p_{m_2}(0) = 0.2$, $p_{m_3}(0) = 0.3$. The growth functions are shown in Figure 1, while the identified values of the kinetic parameters are: $\mu_{m_1}^a = 1.284$day^{-1}, $K_{s_1}^a = 11.297$g/L, $\mu_{m_2}^a = 0.724$day^{-1}, $K_{s_2}^a = 14.291$mmol/L, $K_{i_2}^a = 255.65$mmol/L. The minimum dilution rate has been selected as $u_{min} = 0.3$day^{-1}, which guarantees for the averaged model the convergence to an operational point from any system initial condition characterized by the presence of both bacteria type ($\xi_3^a(0) > 0$, $\xi_4^a(0) > 0$). The maximum dilution rate has been chosen as $u_{max} = 0.49$day^{-1}, which ensures the occurrence of the operational equilibria, while the optimal dilution rate has been calculated as $u_s = 0.4728$day^{-1}. The corresponding optimal steady state of the averaged model is $\xi_s^a = \begin{bmatrix} 6.58 & 36.79 & 0.79 & 0.86 \end{bmatrix}^T$ and the outflow rate of biogas produced in this steady state is $Q(\xi_s^a) = 184.28$L/day.

Table 2 presents the optimal dilution rates and the corresponding maximum biogas outflow rates for each possible combination of the acidogenic and methanogenic species. It is worth noting that, except the cases involving the third methanogenic species, the averaged model predicts a lower biogas outflow rate achievable with a lower dilution rate than the optimal ones calculated for species combination. Note

Table 1: Numerical values of the parameters for the multispecies system - case 1

Stoichiometric	a	42.14	c	116.5 mmol/g
	d	268 mmol/g	q	453 mmol/g
Acidogens	$\mu_{m_1}^1$	1.2 day^{-1}	$K_{s_1}^1$	7.1 g/L
	$\mu_{m_1}^2$	1.56 day^{-1}	$K_{s_1}^2$	21.3 g/L
	$\mu_{m_1}^3$	0.96 day^{-1}	$K_{s_1}^3$	2.13 g/L
Methanogens	$\mu_{m_2}^1$	0.74 day^{-1}	$K_{s_2}^1$	9.28 mmol/L
	$\mu_{m_2}^2$	1.258 day^{-1}	$K_{s_2}^2$	41.76 mmol/L
	$\mu_{m_2}^3$	0.518 day^{-1}	$K_{s_2}^3$	15.776 mmol/L
			$K_{i_2}^1$	256 mmol/L
			$K_{i_2}^2$	128 mmol/L
			$K_{i_2}^1$	384 mmol/L



(a) (b)

Figure 1: Growth functions of the acidogenic and methanogenic species and of the averaged model - case 1

Table 2: Optimal dilution rates / optimal outflow rates of methane for pairs of acidogenic and methanogenic species - case 1

	m_1	m_2	m_3
a_1	0.5179 / 211.005	0.5551 / 208.870	0.3478 / 138.886
a_2	0.5141 / 198.529	0.5469 / 194.431	0.3457 / 133.695
a_3	0.5197 / 218.044	0.5590 / 217.221	0.3488 / 141.639

also that these optimal dilution rates are higher than the selected u_{max}, which indicates that in principle the system can be operated at a higher dilution rate without wash-out occurrence. Therefore, if wash-out occurs, this is a consequence of the species selection process (i.e. the third methanogenic species has been selected) and it is not due to inadequately chosen dilution rates (biomass is washed-out when the system is operated with a dilution rate higher than the maximum of the growth function).

Figure 2 shows the phase portrait of the averaged model (11)-(14) on the plane Δ^a, controlled with the proposed optimization technique. This illustrates the case of a single species system for which an accurate model is available. Figure 2 shows the position of the acidification and the operational steady states for the system operated with u_s, the physical boundaries in continuous lines, the switching curve in dashed line and the target set around the optimal equilibrium. The operation is intuitively represented on the right hand side of the phase portrait for one of the system trajectory originating in an initial state on the physical boundary: the system is operated with u_{min} until the trajectory reaches the switching curve, then the dilution rate is changed to u_{max} and the system is operated with the new value until the target set is reached; in the end the dilution rate is set to the optimal value and the system converges to the optimal setpoint.

Figure 3 shows the phase portrait of the controlled multispecies system (1)-(4), where the total amount of methanogens is plotted against the total amount of acidogens. The steady states of the averaged model for $u = u_s$ are illustrated with circles, while the steady states of the multispecies system corresponding to the winning pair for the same dilution rate are illustrated with squares. All considered trajectories settle down in a meaningful equilibrium point. Figure 4 illustrates the time evolution of the biomasses and the biogas production in the controlled averaged system and in the controlled multispecies system, respectively. The species a_3 wins the competition among the acidogens, while the species m_1 wins the competition among the methanogens. There is no particularity in the species selection process in this case, as for each dilution rate level, the species a_3 and m_1 need the smallest amount of substrates ξ_1 and ξ_2, respectively. This can be seen in Figure 1. Compared to the single species system (illustrated here by the averaged model), the final steady state is reached much faster and higher biogas outflow rate and

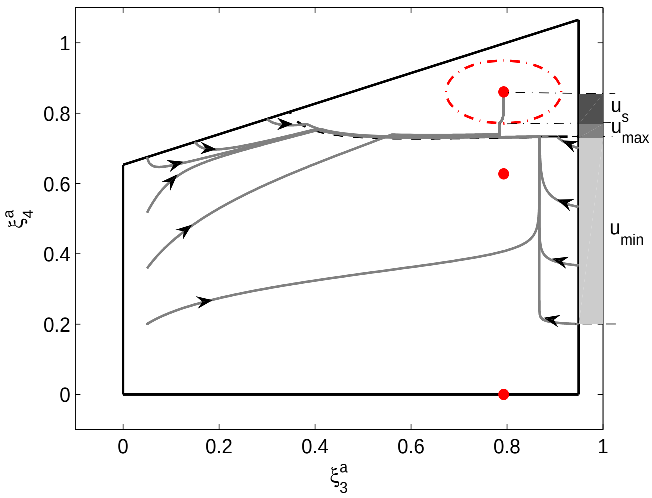


Figure 2: Controlled phase portrait of the averaged model on the plane Δ^a - case 1

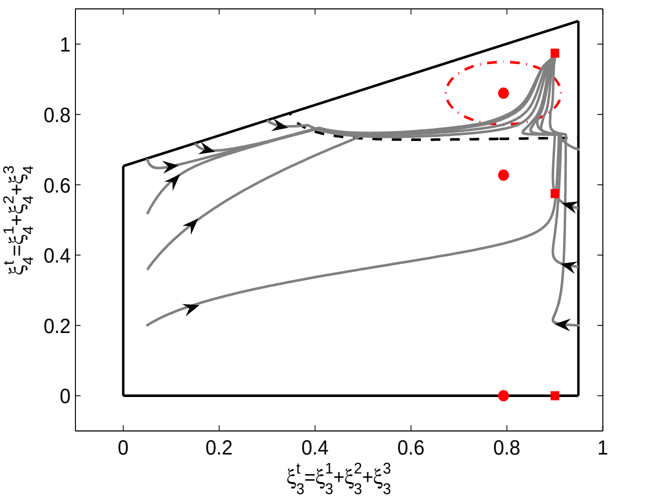


Figure 3: Controlled phase portrait of the multispecies system - case 1

COD consumption are obtained in the multispecies system. According to Table 2, the species combination which leads to the highest biogas production in steady state is the one that was selected using the optimization strategy. However, less biogas is produced due to the fact that the system is operated with the optimal dilution rate computed from the averaged model and not the one given in Table 2.

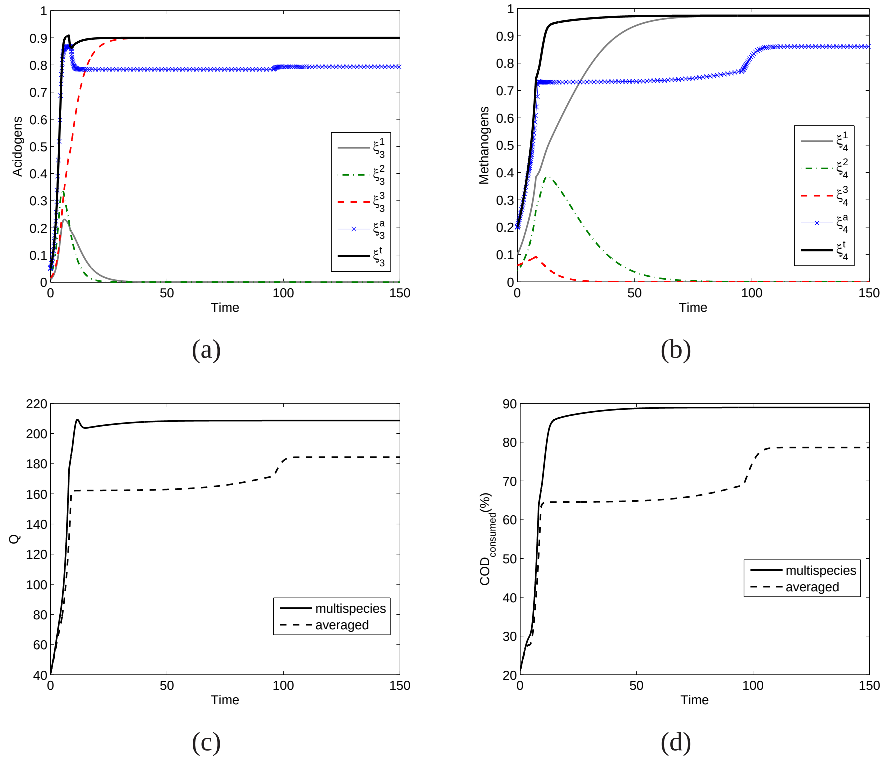


Figure 4: Time evolution of the biomasses, the biogas production and the COD consumption for a controlled trajectory - case 1

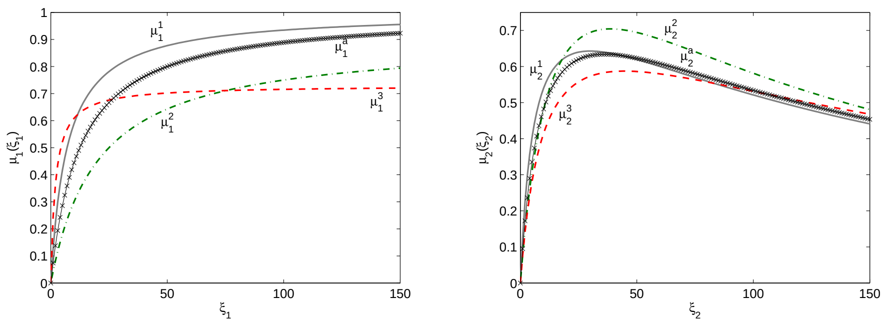
4.2 Inaccurate averaged model

Identifying an accurate averaged model for the multispecies system is a difficult task due to the numerous species composing the ecosystem and the permanent interactions between them. In this section we illustrate the efficiency of the optimization strategy using an averaged model, which is not built based on the relationships (20) and (21) at the initial time $t = 0$. The kinetics of the averaged model shown in Figure 5, have been chosen such that they are of the same order

Table 3: Numerical values of the parameters for the multispecies system - case 2

Acidogens	$\mu_{m_1}^1$	1 day^{-1}	$K_{s_1}^1$	7 g/L
	$\mu_{m_1}^2$	0.9 day^{-1}	$K_{s_1}^2$	20 g/L
	$\mu_{m_1}^3$	0.73 day^{-1}	$K_{s_1}^3$	2 g/L
Methanogens	$\mu_{m_2}^1$	0.9 day^{-1}	$K_{s_2}^1$	6 mmol/L
	$\mu_{m_2}^2$	1.25 day^{-1}	$K_{s_2}^2$	15 mmol/L
	$\mu_{m_2}^3$	0.85 day^{-1}	$K_{s_2}^3$	10 mmol/L
			$K_{i_2}^1$	150 mmol/L
			$K_{i_2}^2$	100 mmol/L
			$K_{i_2}^1$	200 mmol/L

of magnitude as the kinetics of the multispecies system, without assuming any species proportions. The parameters of the averaged model are: $\mu_{m_1}^a = 1$day^{-1}, $K_{s_1}^a = 12.5$g/L, $\mu_{m_2}^a = 0.95$day^{-1}, $K_{s_2}^a = 9$mmol/L, $K_{i_2}^a = 145$mmol/L, while the kinetic parameters of the multispecies system are given in Table 3. For the simulation of the start-up, the proportions have been initially selected as $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.3$, $p_{a_3}(0) = 0.3$, $p_{m_1}(0) = 0.3$, $p_{m_2}(0) = 0.4$, $p_{m_3}(0) = 0.3$.



(a) (b)

Figure 5: Growth functions of the acidogenic and methanogenic species and of the averaged model - case 2

As in the previous case, the minimum dilution rate has been selected as $u_{min} = 0.3$day^{-1}, ensuring thus the convergence of the averaged model to an operational point from any system initial condition characterized by the presence of both bacteria type. The maximum dilution rate has been chosen as $u_{max} = 0.63$day^{-1}, which ensures the occurrence of the operational equilibria, while the optimal dilution rate has been calculated as $u_s = 0.599$day^{-1}. The corresponding optimal steady state of the averaged model is $\xi_s^a = \begin{bmatrix} 18.67 & 20.13 & 0.5 & 0.8 \end{bmatrix}^T$ and the outflow rate of biogas produced in this steady state is $Q(\xi_s^a) = 217.08$L/day.

Table 4: Optimal dilution rates / optimal outflow rates of methane for pairs of acidogenic and methanogenic species - case 2

	m_1	m_2	m_3
a_1	0.6246 / 247.290	0.6665 / 251.830	0.5651 / 222.843
a_2	0.5182 / 176.659	0.5173 / 174.281	0.4971 / 169.316
a_3	0.6057 / 248.671	0.6147 / 247.954	0.5623 / 228.809

Table 4 presents the optimal dilution rates and the corresponding maximum biogas outflow rates for each possible combination of the acidogenic and methanogenic species. Except for the combinations involving the acidogenic species a_2, all the others provide higher biogas outflow rate in steady state than the one predicted by the model. Noticeable in this case is the fact that the optimal dilution rate for the pair a_1-m_2 is higher than u_{max}.

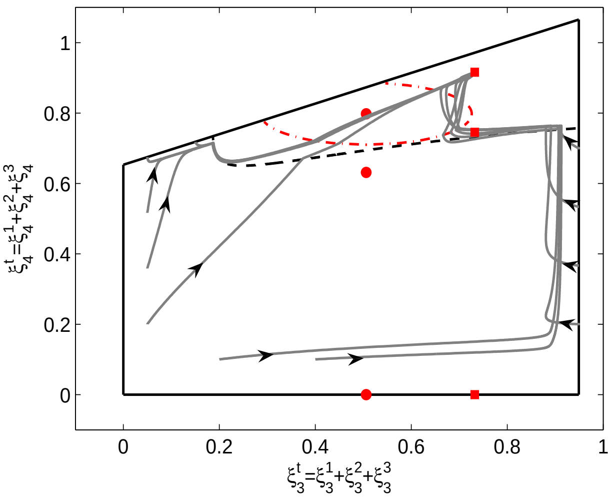


Figure 6: Controlled phase portrait of the multispecies system - case 2

Figure 6 shows the phase portrait of the controlled multispecies system as total amount of acidogens versus total amount of methanogens. The steady states of the averaged model for $u = u_s$ are illustrated with circles, while the steady states of the multispecies system corresponding to the winning pair for the same dilution rate are illustrated with squares. Figure 7 shows the time evolution of the biomasses, the biogas production and the COD consumption in the controlled averaged system and in the controlled multispecies system, respectively. In this case, the different levels of the dilution rate favor different species in the group: for u_{min}, the species a_3 and m_1 are favored, while for u_{max} the species a_1 and

m_2 are promoted. In the end, the species a_3 wins the competition among the acidogens, while the species m_1 wins the competition among the methanogens as they require the smallest amount of ξ_1 respectively ξ_2 for u_s. This may be noticed in Figure 5. Now, the species selection process is slower than the averaged model dynamics due to the small difference in the break-even concentrations of the species a_1 and a_3 and of the species m_1 and m_2; however, the biogas outflow rate and the COD consumption reach levels very close to their steady states as fast as the averaged model. In steady state, the biogas outflow rate produced by the multispecies system is very close to the optimal value of the pair a_3-m_1, as the optimal dilution rate for this pair and u_s, the optimal dilution rate of the averaged model, assume similar values (see Table 4).

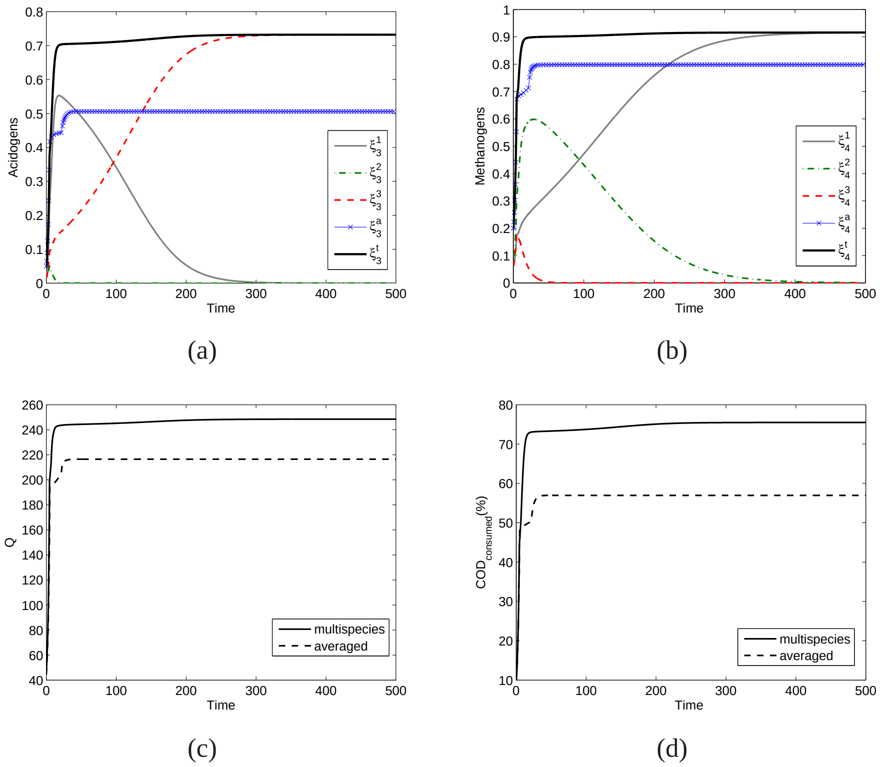


Figure 7: Time evolution of the biomasses and the biogas production for a controlled trajectory - case 2

4.3 Discussion

The simulation results presented in the previous section for both the accurate and inaccurate averaged models show that in all cases a meaningful steady state is reached, characterized by a higher biogas outflow rate (very close to the maximal one) and higher COD consumption than the ones predicted by the averaged model. An important question is whether or not the start-up procedure leads to the selection of the most efficient species in terms of biogas production. It can be proven (see Appendix A), using the analytical expressions of the equilibrium points, that the acidogenic and methanogenic species winning the competition for $u = u_s$ are the most efficient ones at this dilution rate among the species present in the reactor. These are the species needing the smallest amount of substrates in steady state, which implies a high treatment efficiency as the amount of untreated organic mater (substrates leaving the reactor) is at the lowest possible level. The amount of biogas produced in steady state is given by the product between $q \cdot u_s$ and the concentration of methanogenic bacteria winning the competition. This concentration is the highest among all methanogenic species (see the expression of system equilibria in [6]), which implies that the biogas outflow rate is maximum. Note that the species efficiency is evaluated with respect to the dilution rate levels chosen on the basis of the averaged model. In reality, higher biogas outflow rate for a higher dilution rate could be obtained by selecting another pair of species, such as a_1-m_2 in Table 4. However, kinetics of the individual species are not available in practice, the only known kinetics are the ones of the identified averaged model. We conclude that the competitive exclusion is the best selection process of the most efficient species in generating the highest amount of biogas at the dilution rate u_s. However, a crucial condition is that these species are present in the reactor in the final stage of the control strategy, i.e., they have not been washed-out before switching the dilution rate to u_s. Another important aspect is that their concentration must be high enough such that the wash-out of all methanogenic species does not occur while trying to select the best suited species for biogas production. Hence, a study regarding the long run coexistence of the species, such as the one presented in [12] for species with Monod kinetics, is necessary to estimate the time the species coexist and eventually adjust the switching moments for the dilution rate accordingly. This may be also the solution to prevent the total wash-out of the methanogens.

5 Identifying possible causes for the failure of the start-up

The simulation results presented in the previous section indicate that the start-up strategy will work in possibly many situations independently of the accuracy of the averaged (at the initial time) model. In the absence of a rigorous mathematical study to provide conditions for a successful start-up, we proceed by investigating in simulation in which circumstances failure of the start-up may occur.

The cause determining the failure of the start-up is the combined effect of switching the dilution rate to the maximum level u_{max} and the initial species proportions. When the same species in the group is promoted for each of the three levels of the dilution rate (such as in case 1 in the previous section), it is straightforward to conclude that a high enough initial proportion of this species helps preventing the wash-out when the dilution rate is changed from u_{min} to u_{max}, implying thus a safe start-up of the process. The reasonably high initial proportion of the favored species counteracts the contribution of the other species in the total biomass (which is used as an indicator for switching the dilution rate), ensuring a high concentration of the promoted species at the switching instant.

When various species in the group are favored at different dilution rate levels, the role of the initial species proportions is not so evident. Further on we consider the example given in case 2 in the previous section and we simulate the start-up for various initial proportions of the species in order to determine their influence. The most efficient species for biogas production, winning the competition for the dilution rate u_s are the acidogens a_3 and the methanogens m_1. These species are also favored for the system operation with the dilution rate u_{min}; for the operation with the dilution rate u_{max} the promoted species are a_1 and m_2.

Figure 8 shows the controlled phase portrait of the multispecies system as total amount of acidogens versus total amount of methanogens when the initial species proportions are: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.05$, $p_{m_2}(0) = 0.45$, $p_{m_3}(0) = 0.5$. These have been selected such that the winning species a_3 and m_1 have the smallest initial proportions compared to the ones of the competitors in the group. Each system trajectory converges to the desired operating point, showing a successful start-up of the system. Therefore, in situations like the one illustrated here, high initial proportions of the winning species in the final stage is not a prerequisite for a safe start-up.

Figure 9 illustrates the controlled phase portrait of the multispecies system for another initial distribution of the species: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.5$, $p_{m_2}(0) = 0.2$, $p_{m_3}(0) = 0.3$. Compared to the previous case, the initial proportion of the species m_1 has been increased to the detriment of the proportions of m_2 and m_3. Now, some of the system trajectories converge to

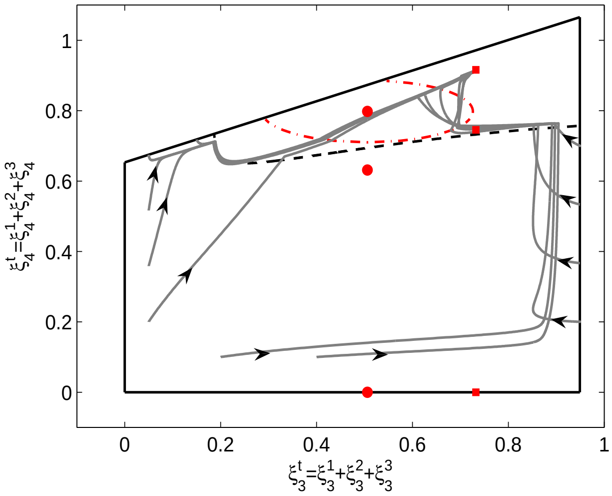


Figure 8: Controlled phase portrait of the multispecies system: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.05$, $p_{m_2}(0) = 0.45$, $p_{m_3}(0) = 0.5$

the methanogens wash-out, showing that the start-up can fail even if a reasonably high concentration of the winning species is initially available. The set of initial conditions from where the system is driven to wash-out increases even more when the initial proportion of m_3, the species which is never promoted in this example, is the highest: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.3$, $p_{m_2}(0) = 0.2$, $p_{m_3}(0) = 0.5$. As Figure 10 shows, the start-up is successful in this case only if the system starts in two particular initial states among the considered ones.

These simulation results indicate that for multispecies systems where different species are favored for the three dilution rate levels, the successful application of the proposed start-up strategy is highly dependent on the initial species distribution. Of particular importance is the fact that although competing with the others, the species promoted for the dilution rate u_{max} is supporting the system start-up: unless it has a reasonably high concentration, the start-up will fail due to the methanogenic bacteria wash-out.

In the theoretical scenario of measuring the total biomass and the two substrates (as considered throughout this paper), one way to prevent the failure of the start-up strategy is to consider multiple switch of the dilution rate between the minimum and maximum levels at any time the system state moves on the other side of the switching surface. This will re-launch the competition among the species and possibly lead to the selection of an acidogenic and a methanogenic species, when the switch to the optimal dilution rate level u_s occurs. A more practical approach is to consider the measurement of biogas and switch between

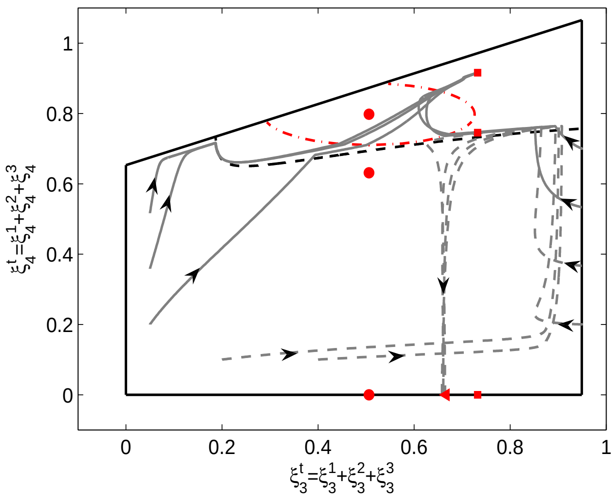


Figure 9: Controlled phase portrait of the multispecies system: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.5$, $p_{m_2}(0) = 0.2$, $p_{m_3}(0) = 0.3$

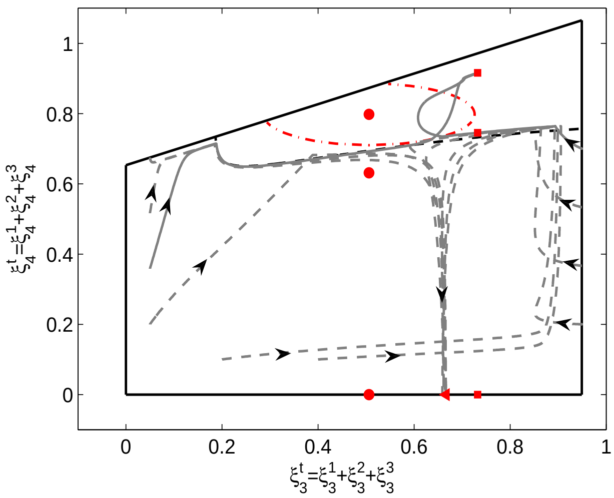


Figure 10: Controlled phase portrait of the multispecies system: $p_{a_1}(0) = 0.4$, $p_{a_2}(0) = 0.5$, $p_{a_3}(0) = 0.1$, $p_{m_1}(0) = 0.3$, $p_{m_2}(0) = 0.2$, $p_{m_3}(0) = 0.5$

the minimum and maximum dilution rates whenever biogas production decreases. It has been shown that the outflow rate of biogas is a good indicator of biomass growth [13, 14].

6 Conclusions

In this paper a brief evaluation of a start-up policy for multispecies anaerobic digestion systems is presented, where the implementation of the strategy developed for single species systems makes use of an averaged model. This model is constructed so as to represent in an average sense the kinetics of the global population at the initial time. However, as the system operation proceeds, the averaged kinetics and the real ones are differing sometimes considerably. The simulation results obtained using both accurate and inaccurate averaged kinetics indicate that this strategy leads to a consolidated ecosystem, with enhanced productivity compared to the one predicted by the averaged model and very close to the maximal one of the multispecies system. There are also cases when the start-up will fail, due to the initial species distribution. However, further investigations are needed to have a complete view on the necessary conditions for the successful start-up of the multispecies system. Of particular importance is the estimation of the time span the species can coexist in the reactor, which may play a prominent role in some cases for the selection of the most efficient species.

Acknowledgement

This paper presents research results of the Belgian Network DYSCO (Dynamical Systems, Control, and Optimization), funded by the Interuniversity Attraction Poles Programme, initiated by the Belgian State, Science Policy Office. The scientific responsibility rests with its author(s).

A Proof of the most efficient species selection at the optimal dilution rate

The equilibrium state reached by the multispecies system for the operation with the constant dilution rate $u = u_s$ has the form

$$\xi^s = \begin{bmatrix} \xi_1^s \\ \xi_2^s \\ \xi_3^s \\ \xi_4^s \end{bmatrix} \tag{22}$$

with

$$\xi_3^s = \begin{bmatrix} 0 & \dots & \xi_3^{k,s} & \dots & 0 \end{bmatrix}^T, \quad \xi_4^s = \begin{bmatrix} 0 & \dots & \xi_4^{l,s} & \dots & 0 \end{bmatrix}^T$$

where $\xi_3^{k,s}$, $\xi_4^{l,s}$ denote the acidogenic and methanogenic species winning the competition at $u = u_s$, respectively. Hence, $\xi_1^s = \xi_1^{k,s}$ is the unique solution of

$$\mu_1^k(\xi_1) = u_s \tag{23}$$

while $\xi_2^s = \xi_2^{l,s}$ is the smaller solution of

$$\mu_2^l(\xi_2) = u_s \tag{24}$$

Since the winning species are the ones requiring the smallest amount of nutrient, then

$$\xi_1^{k,s} = \min\left\{\xi_1^{i,s}, \quad i = 1 \dots n\right\} \tag{25}$$

$$\xi_2^{l,s} = \min\left\{\xi_2^{j,s}, \quad j = 1 \dots m\right\} \tag{26}$$

with $\xi_1^{i,s}$, $\xi_2^{j,s}$ solutions of equations similar to (23), (24), respectively. According to [6],

$$\xi_3^{k,s} = \left(\xi_{in_1} - \xi_1^{k,s}\right)/a \tag{27}$$

$$\xi_4^{l,s} = \left(\xi_{in_2} - \xi_2^{l,s} + c\xi_3^{k,s}\right)/d \tag{28}$$

As ξ_{in_1}, ξ_{in_2} are constant, using (25), (26) in (27), (28) leads to

$$\xi_3^{k,s} = \max\left\{\xi_3^{i,s}, \quad i = 1 \dots n\right\} \tag{29}$$

$$\xi_4^{l,s} = \max\left\{\xi_4^{j,s}, \quad j = 1 \dots m\right\} \tag{30}$$

Since the amount of biogas produced in steady state is proportional to the product between the dilution rate u_s and the concentration of the winning methanogenic species, using (30) it is straightforward to conclude that the most efficient species combination for biogas production has been selected.

References

[1] C. Delbès and R. Moletta and J.-J. Godon, *Bacterial and archaeal 16s rdna and 16s rrna dynamics during an acetate crisis in an anaerobic digestor ecosystem*, FEMS Microbiology Ecology 35 (2001), pp. 19–26.

[2] P. Masci and O. Bernard and F. Grognard and E. Latrille and J.-B. Sorba and J.-P. Steyer,*Driving competition in a complex ecosystem: application to anaerobic digestion*, in *Proceedings of the ECC Conference*, Budapest, Hungary, 2009.

[3] M. Sbarciog and M. Loccufier and A. Vande Wouwer, *On the Optimization of Biogas Production in Anaerobic Digestion Systems*, in *Preprints of the 18th IFAC World Congress*, Milan, Italy, 2011, pp. 7150–7155.

[4] M. Sbarciog and M. Loccufier and A. Vande Wouwer, *An Optimizing Start-up Strategy for a Bio-methanator*, Bioprocess Biosyst Eng 35, (2012), pp. 565–578.

[5] O. Bernard and Z. Hadj-Sadok and D. Dochain and A. Genovesi and J. P. Steyer, *Dynamical model development and parameter identification for an anaerobic wastewater treatment process*, Biotechnology and Bioengineering 75 (2001), pp. 424–438.

[6] M. Sbarciog and M. Loccufier and E. Noldus, *Determination of appropriate operating strategies for anaerobic digestion systems*, Biochemical Engineering Journal 51 (2010), pp. 180–188.

[7] G. Hardin, *The competition exclusion principle*, Science 131 (1960), pp. 1292–1298.

[8] H.L. Smith and P. Waltman, *The theory of the chemostat. Dynamics of microbial competition*, Cambridge University Press, Cambridge, 1995.

[9] G.J. Butler and G.S.K. Wolkowicz, *A mathematical model of the chemostat with a general class of functions describing nutient uptake*, SIAM J. Appl. Math. 45 (1985), pp. 138–151.

[10] M. Sbarciog and M. Loccufier and E. Noldus, *The computation of stability boundaries in state space for a class of biochemical engineering systems*, J. Computational and Applied Mathematics 215, 2008, pp. 557–567.

[11] M. Sbarciog and M. Loccufier and E. Noldus, *The estimation of stability boundaries for an anaerobic digestion system*, in *Proceedings of the 11th International Symposium on Computer Applications in Biotechnology*, Leuven, Belgium, 2010, pp. 359–364.

[12] A. Rapaport and D. Dochain and J. Harmand, *Long run coexistence in the chemostat with multiple species*, Journal of Theoretical Biology 257 (2009), pp. 252–259.

[13] M. Sbarciog and J.A. Moreno and A. Vande Wouwer, *A biogas-based switching control policy for anaerobic digestion systems*, in *Proceedings of the 8th IFAC Symposium on Advanced Control of Chemical Processes*, Singapore, 2012, pp. 603–608.

[14] M. Sbarciog and J.A. Moreno and A. Vande Wouwer, *Simple approaches to start-up anaerobic digestion systems for biogas production*, in *Proceedings of ICSTC*, Sinaia, Romania, 2012.