

Transient Analysis of a Two-Level Controller for an Anaerobic Bioreactor

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Abstract: We consider a mechanistic mathematical model of an anaerobic bioreactor, where the controlled input is the dilution rate and the measured output is the methane outflow rate. A steady-state and transient analysis is made to prove that when the dilution rate is alternated between two values, one below and one above the unknown optimal steady-state maximizing value, the output signal reaches temporary maxima that could be used for driving the feedback. A simulation example illustrates the findings and discusses the limitations.

Keywords: Biotechnology, transient analysis, output feedback, extremum seeking

1. INTRODUCTION

In Mexico there is growing concern for the decrease in the current fossil fuel production and our dependence on it for producing energy (SEMARNAT-INECC, 2016). Research on alternative fuels from renewable sources is an important current topic, and one of them is biogas, which is the product of the fermentation of a host of biobased materials, notably including wastes (OECD/IEA, 2016).

A widely used process used for converting liquid waste into biogas is anaerobic digestion. In this process, a consortia of microorganisms degrade the organic matter present in the waste stream by a set of interconnected biochemical reactions carried out by specialized microorganisms. In the final stages of the process, a product is biogas, composed mainly of methane (CH_4) and carbon dioxide (CO_2), but also other gases in trace amounts such as hydrogen sulfide (H_2S) or hydrogen (H_2). This biogas is a valuable renewable fuel that can be used directly for powering electrical generators or purified into biomethane to be injected to a natural gas network. The waste feed stream may be high strength wastewater, excess sludge from wastewater treatment, or the organic fraction of municipal solid waste, among others (Batstone, 2006).

One of the main concerns when operating an anaerobic digester is maintaining a stable operation, with constant and adequate biogas production while achieving good treatment standards, despite the inevitable changes in the waste stream that is fed, both in composition and concentration. A mathematical model of the process may aid in the design of a feedback controller that not only stabilizes the system, but also helps achieve near maximal biogas productivity (Batstone, 2006).

The anaerobic digestion process is very complex, but can be well and quite accurately described by models such the Anaerobic Digestion Model 1 (ADM1) (Batstone et al., 2002). However, this model is still too complex for analysis and model-based controller design and simpler models

have been proposed, such as the AM2 model (Bernard et al., 2001), which is composed of four differential equations and captures the basic dynamics of the process. Numerous studies have used it as a basis for system analysis and controller proposals (Antonelli et al., 2003; Sbarciog et al., 2012). However, it suffers from several drawbacks when compared to the accuracy of the ADM1, especially when the substrate is complex and there is an interest in predicting the physicochemistry of the process. Recently, Hassam et al. (2015) have proposed the AM2HN model, which now includes a hydrolysis step and better predictions of the pH and the alkalinity, comparable to ADM1.

In this work, based on the transient analysis of the AM2HN model, we propose a simple feedback controller that switches between operation at a low and a high dilution rate in order to practically maximize the methane production rate. The main asset of this proposal is that it does not depend directly on the knowledge of model parameters, and is based on the qualitative behavior of a realistically measurable output signal.

The paper is organized as follows. The next section introduces the mathematical model used, i.e. the AM2HN, followed by the idea behind a controller for maximizing the methane flow rate and a steady-state analysis. The next section analyzes the transient when the dilution rate changes from a low to a high value and viceversa. This is followed by simulation results and a conclusion.

2. MATHEMATICAL MODEL

The model considers three basic biochemical reactions: hydrolysis, acidogenesis and methanogenesis, as well as biomass decay. The components in the liquid phase are: particulate substrate X_T , soluble substrate S_1 , volatile fatty acids (VFA) S_2 , acidogenic biomass X_1 , methanogenic biomass X_2 , inorganic carbon C (dissolved carbon dioxide and bicarbonate) and alkalinity Z . In the gas phase only methane (CH_4) and carbon dioxide (CO_2) are considered; gas transfer equations are needed to model their behavior.

Furthermore, the physicochemistry of speciation is used algebraically to calculate the pH.

The model differential equations are the following:

$$\dot{X}_1 = -X_1 \alpha D + (\mu_1(S_1) - k_{d1}) X_1 \quad (1)$$

$$\dot{X}_2 = -X_2 \alpha D + (\mu_2(S_2) - k_{d2}) X_2 \quad (2)$$

$$\dot{X}_T = (X_T^{in} - X_T) D - k_{hyd} X_T \quad (3)$$

$$\dot{S}_1 = (S_1^{in} - S_1) D - k_1 \mu_1(S_1) X_1 + k_{hyd} X_T \quad (4)$$

$$\dot{S}_2 = (S_2^{in} - S_2) D + k_2 \mu_1(S_1) X_1 - k_3 \mu_2(S_2) X_2 \quad (5)$$

$$\dot{C} = (C^{in} - C) D + k_4 \mu_1(S_1) X_1 + k_5 \mu_2(S_2) X_2 - q_c \quad (6)$$

$$\dot{Z} = (Z^{in} - Z) D + k_1 N_{S1} \mu_1(S_1) X_1 - N_{bac} ((\mu_1(S_1) - k_{d1}) X_1 + (\mu_2(S_2) - k_{d2}) X_2) \quad (7)$$

A factor $\alpha \in [0, 1]$ is considered for accounting for partial biomass retention in the reactor ($\alpha = 1$ corresponds to a CSTR and $\alpha = 0$ to perfect retention). The specific reaction rates are of Monod type for acidogenesis and Haldane type for methanogenesis:

$$\mu_1(S_1) = \frac{\mu_1^* S_1}{K_{S1} + S_1}, \quad (8)$$

$$\mu_2(S_2) = \frac{\mu_2^* (S_2/S_2^*)}{S_2/S_2^* + \beta (S_2/S_2^* - 1)^2}, \quad (9)$$

where in the Haldane law the maximum occurs at (S_2^*, μ_2^*) and the slope at $S = 0$ is $\mu_2'(0) = \mu_2^*/(\beta S_2^*)$. Total alkalinity Z is considered as the sum of the concentrations of all bases in solution. This corresponds basically to bicarbonate (HCO_3^-), dissociated VFA (S_2^-), and free ammonia (NH_3). In this model, for simplicity, ammoniacal nitrogen is not included as a component, but the nitrogen release dynamics is included by making alkalinity a reactive species. Ammonium (NH_4^+) is released from protein hydrolysis and three components contain nitrogen: the degradable substrate S_1 whose nitrogen content is N_{S1} (mmolN/gCOD), and the acidogenic X_1 and methanogenic X_2 biomasses, whose nitrogen content is N_{bac} (mmolN/gCOD). Alkalinity is decreased by biomass decay and substrate uptake (due to ammonium release), but increased by biomass growth (due to nitrogen uptake).

Soluble methane is produced in methanogenesis and its gaseous outflow rate is assumed to be proportional to the methane production rate:

$$q_m = k_6 \mu(S_2) X_2. \quad (10)$$

On the other hand, the rate of carbon dioxide transfer to gas phase follows Henry's law:

$$q_c = k_L a (C_{co2} - K_H P_c), \quad (11)$$

where $k_L a$ is the liquid-gas transfer coefficient, K_H is Henry's constant, C_{co2} is the dissolved CO_2 concentration in the liquid and P_c is the partial pressure of carbon dioxide in the gas phase, calculated using (Hassam et al., 2015)

$$P_c = \Phi - \sqrt{\Phi^2 - P_{gas} \frac{C_{co2}}{K_H}}, \quad (12)$$

$$\Phi = \frac{1}{2} \left(P_{gas} + \frac{C_{co2}}{K_H} + \frac{q_m}{k_L a K_H} \right), \quad (13)$$

where usually $P_{gas} = P_{atm}$ and C_{co2} depends on the pH. To calculate it, we must solve a system of algebraic equations based on the acid-base equilibrium equations.

Basically, we must first solve for pH the following algebraic equation:

$$Z + 10^{-pH} = \frac{C}{1 + 10^{pK_c - pH}} + \frac{S_2}{1 + 10^{pK_a - pH}} + 10^{pH - pK_w},$$

where $pK_c = 6.31$, $pK_a = 4.77$, $pK_w = 13.68$ are the pK values for the inorganic carbon, VFA and water acid-base pairs. Finally, the amount of C_{co2} is obtained from

$$C_{co2} = \frac{C}{1 + 10^{pH - pK_c}}. \quad (14)$$

3. CONTROLLER PROPOSAL

The objective is to maximize the methane flow rate, i.e. q_m , by manipulating the dilution rate D . A steady-state analysis shows that indeed, if the influent substrate concentrations X_T^{in} , S_1^{in} , S_2^{in} are constant, there is an optimal D_{opt} that maximizes q_m in steady-state. However, in practice we are faced with two problems. First, the value of D_{opt} depends on the values of X_T^{in} , S_1^{in} , S_2^{in} , which might be unknown, and even if we could measure these concentrations, we might need to know the model exactly (i.e. all its parameters) to compute D_{opt} . Secondly, in practice the influent substrate concentrations are slowly time-varying and the parameters' values could have some drift or uncertainty. This means that usually the input/output steady state map is unknown, and therefore extremum-seeking feedback control strategies for this type of systems have been proposed recently (Wang et al., 1999; Dieulot, 2012; Lara-Cisneros et al., 2014). However, they converge very slowly, because they imply reaching quasi-steady-state conditions.

We tackle the extremum-seeking problem differently. Instead of waiting for a quasi-steady-state, we take advantage of the qualitative transient behavior of a suitable output measurable signal upon sudden changes in the input variable, i.e. $D(t)$. In fact, we claim that by alternating between two values of D , one surely below and another one surely above D_{opt} , we obtain an output signal that will oscillate around the maximum of q_m . To prove it we first make a steady-state analysis of the system (1)–(14) and then analyze the transient behavior.

4. STEADY-STATE ANALYSIS

For a constant dilution rate D , and constant influent concentrations S_1^{in} , S_2^{in} , X_T^{in} , C^{in} and Z^{in} , the system may have up to five operating points, some of them stable and some of them unstable. However, if we assume some realistic parameter values, we can focus the analysis on only some conditions. Notice that (3) is decoupled from the rest of the system, so its steady state is simply¹:

$$\bar{X}_T = \frac{D}{k_{hyd} + D} X_T^{in}. \quad (15)$$

The steady state for alkalinity $\bar{Z}$ is obtained directly from (7) if the other values for the steady states have been computed. Likewise, we can compute the unique solution for inorganic carbon $\bar{C}$ from solving (6) and the algebraic equations (11)–(14).

¹ We use the notation $\bar{\cdot}$ as in $\bar{X}_1$ to denote the steady-state value.

We only then analyze the steady states of subsystem (X_1, X_2, S_1, S_2) , given $\bar{X}_T$. This analysis would be practically the same as the one already reported for the AM2 model (Volcke et al., 2010), substituting S_1^{in} by

$$S_1^{max} = S_1^{in} + \frac{k_{hyd}}{k_{hyd} + D} X_T^{in}. \quad (16)$$

Assuming that D satisfies $(k_{d1} + \alpha D) \leq \mu_1(S_1^{max})$, then apart from the washout $\bar{X}_1 = 0$, $\bar{S}_1 = S_1^{max}$, there is another equilibrium point satisfying

$$\mu_1(\bar{S}_1) = k_{d1} + \alpha D, \quad \bar{X}_1 = \frac{(S_1^{max} - \bar{S}_1) D}{k_1 (k_{d1} + \alpha D)} \quad (17)$$

Now define

$$S_2^{max} = S_2^{in} + \frac{k_2}{k_1} (S_1^{max} - \bar{S}_1). \quad (18)$$

Consider the solution(s) $\bar{X}_2 > 0$, $\bar{S}_2 > 0$, satisfying

$$\mu_2(\bar{S}_2) = k_{d2} + \alpha D, \quad \bar{X}_2 = \frac{(S_2^{max} - \bar{S}_2) D}{k_3 (k_{d2} + \alpha D)} \quad (19)$$

There will be no solution if $(k_{d2} + \alpha D) > \mu_2^*$, two solutions if $\mu_2(S_2^{max}) \leq (k_{d2} + \alpha D) < \mu_2^*$, and only one valid solution if $0 < (k_{d2} + \alpha D) < \mu_2(S_2^{max})$ or if exactly $(k_{d2} + \alpha D) = \mu_2^*$. In any case, it can be shown that only the solution with $\bar{S}_2 < S_2^*$ corresponds to a stable steady state.

We now make the following assumptions on the parameters and inflow concentrations:

- (1) X_T^{in} , S_1^{in} and/or S_2^{in} are such that $S_2^{max} > S_2^*$;
- (2) $\mu_1(S_1^{max}) - k_{d1} > \mu_2^* - k_{d2} > \mu_2(S_2^{max}) - k_{d2} \geq 0$, which implies that the washout condition for methanogens X_2 occurs before the washout of acidogens X_1 if D is gradually increased.

These assumptions imply that as D is increased, we can have one or two stable equilibria depending on the following critical values for D

$$D_{cr1} = \frac{\mu_2(S_2^{max}) - k_{d2}}{\alpha}, \quad D_{cr2} = \frac{\mu_2^* - k_{d2}}{\alpha}, \quad (20)$$

$$D_{cr3} = \frac{\mu_1(S_1^{max}) - k_{d1}}{\alpha}, \quad D_{cr1} < D_{cr2} < D_{cr3}$$

- (1) When $0 \leq D \leq D_{cr1}$, then the only stable equilibrium point happens for $\bar{\xi}_a = (\bar{X}_1, \bar{X}_2, \bar{S}_1, \bar{S}_2)$, cf. (17)–(19).
- (2) When $D_{cr1} < D \leq D_{cr2}$, then bistability occurs with $\bar{\xi}_a$ and methanogens washout: $\bar{\xi}_b = (\bar{X}_1, 0, \bar{S}_1, S_2^{max})$.
- (3) When $D_{cr2} < D < D_{cr3}$, the only stable steady state is the washout of methanogens with $\bar{\xi}_b$.
- (4) When $D \geq D_{cr3}$, the unique stable steady state is the total washout of biomass: $\bar{\xi}_c = (0, 0, S_1^{max}, S_2^{max})$.

Consider that the output is q_m and the desired steady state $\bar{\xi}_a$. Then, from (19)

$$\bar{q}_m = k_6 \mu_2(\bar{S}_2) \bar{X}_2 = \frac{k_6}{k_3} (S_2^{max} - \bar{S}_2) D. \quad (21)$$

Let S_2^{min} satisfy $\mu_2(S_2^{min}) = k_{d2}$. Using (19), we can write (21) as a function of $\bar{S}_2$, with :

$$\bar{q}_m(\bar{S}_2) = \frac{k_6}{\alpha k_3} (S_2^{max} - \bar{S}_2) (\mu_2(\bar{S}_2) - k_{d2}) \quad (22)$$

In the domain $\bar{S} \in [S_2^{min}, S_2^*]$, $f_1(\bar{S}) = S_2^{max} - \bar{S}_2$ is a monotonic decreasing function satisfying

$$f_1 > 0, \quad f_1' = -1 < 0, \quad f_1(S_2^{min}) > 0. \quad (23)$$

Also, $f_2(\bar{S}) = \mu_2(\bar{S}_2) - k_{d2}$ is monotonic increasing with $f_2 > 0, \quad f_2' > 0, \quad f_2(S_2^{min}) = 0, \quad f_2'(S_2^*) = 0. \quad (24)$

This implies that $q_m(\bar{S}) = \frac{k_6}{\alpha k_3} f_1(S_2) f_2(S_2)$ achieves a maximum for some $\bar{S}_2^{opt} < S_2^*$. To see this, notice that $q_m'(S_2^{min}) > 0$ and $q_m'(S_2^*) < 0$, so therefore $q_m'(\bar{S}_2^{opt}) = 0$ at a unique point $\bar{S}_2^{opt} \in [S_2^{min}, S_2^*]$. Since the relationship between D and $\bar{S}$ is injective, cf. (19), for this limited domain, the corresponding $D_{opt} < D_{cr2}$ is also unique.

Obviously, if the influent concentrations change or the parameters drift, the values of D_{opt} , D_{cr1} , D_{cr2} and D_{cr3} change, too. However, it may be possible to choose two values D_{lo} and D_{hi} such that we can guarantee that

$$0 < D_{lo} < D_{opt}, \quad D_{cr2} < D_{hi} < D_{cr3} \quad (25)$$

In the following transient analysis we show that qualitatively, if $D(t)$ is changed from D_{lo} to D_{hi} or if it is changed from D_{hi} to D_{lo} , a transient maximum will occur in the signal $q_m(t)$. However, care should be taken to ensure that the latter change is made when the state trajectory is still in the stability region of the desired equilibrium $\bar{\xi}_a$, since bistability might be present (when $D = D_{lo}$).

5. TRANSIENT ANALYSIS

We will analyze the 5D subsystem (1)–(5), since the other two states are decoupled, but the analysis will be made reducing it to 2D subsystems.

Let $y_{lo}(t; \xi_0)$ be the trajectory of $y(t) = q_m(t)$ under the constant dilution rate D_{lo} when the initial condition is ξ_0 , and likewise, let $y_{hi}(t; \xi_0)$ be the trajectory under the constant dilution rate D_{hi} when the initial condition is ξ_0 . The same notation is meant for the trajectories for the states: $\xi_{lo}(t; \xi_0)$ and $\xi_{hi}(t; \xi_0)$. Furthermore, the stable steady state for D_{hi} is the methanogens washout $\bar{\xi}_b^{hi}$ and for D_{lo} it is $\bar{\xi}_a^{lo}$ and possibly (if $D_{lo} > D_{cr1}$) also $\bar{\xi}_b^{lo}$. This implies that $\lim_{t \rightarrow \infty} y_{hi}(t; \xi_0) = 0$ for any ξ_0 . For D_{lo} , define $\mathcal{R}_{lo}$ as the stability region such that $\xi_0^{lo} \in \mathcal{R}_{lo}$ implies $\lim_{t \rightarrow \infty} \xi_{lo}(t; \xi_0^{lo}) = \bar{\xi}_a^{lo}$.

Theorem 1. There exist a set of parameter values of system (1)–(5) and influent concentrations such that the following is true:

- Consider ξ_0^{hi} such that $\|\xi_0^{hi} - \bar{\xi}_a^{lo}\| < \epsilon$ for some $\epsilon > 0$. There exists $t_{max}^{hi} > t_0$ such that $y_{hi}(t_{max}^{hi}; \xi_0^{hi})$ is maximum with respect to t ; that is $\dot{y}_{hi}(t_{max}^{hi}; \xi_0^{hi}) = 0$ and $\ddot{y}_{hi}(t_{max}^{hi}; \xi_0^{hi}) < 0$.
- Let $T_{hi} > t_{max}^{hi}$, and thus $y_{hi}(T_{hi}; \xi_0^{hi}) < y_{hi}(t_{max}^{hi}; \xi_0^{hi})$ and let $\xi_0^{lo} = \xi_{hi}(T_{hi}; \xi_0^{hi}) \in \mathcal{R}_{lo}$. Then there will also exist t_{max}^{lo} such that $y_{lo}(t_{max}^{lo}; \xi_0^{lo})$ is maximum with respect to t and eventually, when $t = T_{lo} > t_{max}^{lo}$, $\xi_{lo}(t; \xi_0^{lo})$ will reach the ball $\|\xi_{lo} - \bar{\xi}_a^{lo}\| < \epsilon$.

To prove the theorem, consider that (3) is linear when D is constant. If D changes from D_{lo} to D_{hi} and viceversa, then $X_T(t)$ will eventually reach a region bounded by $\bar{X}_T^{lo}$ and $\bar{X}_T^{hi}$. The transient $X_T(t)$ will be exponential with rate $(k_{hyd} + D_{lo})$ or $(k_{hyd} + D_{hi})$. Furthermore, if $k_{hyd} \gg D_{hi}$, then $\bar{X}_T^{hi}$ and $\bar{X}_T^{lo}$ will be small, cf. (15).

Define $S_1^m(t)$ as

$$S_1^m(t) = S_1^{in} + \frac{k_{hyd}}{D} X_T(t). \quad (26)$$

When we change from D_{lo} to D_{hi} and back, S_1^m will be bounded:

$$S_1^{in} + \frac{k_{hyd}}{k_{hyd} + D_{hi}} X_T^{in} < S_1^m(t) < S_1^{in} + \frac{k_{hyd}}{k_{hyd} + D_{lo}} X_T^{in}.$$

We can therefore write (4) as follows:

$$\dot{S}_1 = (S_1^m - S_1) D - k_1 \rho_1 \quad (27)$$

where $\rho_1 = \mu_1(S_1)X_1$. Then $\dot{\rho}_1 = \mu_1 \dot{X}_1 + \mu_1' X_1 \dot{S}_1$ and $\dot{\rho}_1 = X_1 (\mu_1 (\mu_1 - k_{d1} - \alpha D) + \mu_1' ((S_1^m - S_1) D - k_1 \rho_1))$

$$= \rho_1 \left(\mu_1 - k_{d1} - \alpha D + \frac{\mu_1'}{\mu_1} ((S_1^m - S_1) D - k_1 \rho_1) \right) \quad (28)$$

Equations (27)-(28) comprise an approximate 2D system which we can analyze on the phase plane qualitatively. It shows (see similar procedure below) that when $D(t)$ alternates between D_{lo} and D_{hi} , $S_1(t)$, then $\rho_1(t)$ will oscillate between two values (there is no X_1 washout since $D_{hi} < D_{cr3}$). Particularly, if S_1^m is large enough, then

$$(S_1^m(t) - \bar{S}_1^{lo}) \frac{D_{lo}}{k_1} < \rho_1(t) < (S_1^m(t) - \bar{S}_1^{hi}) \frac{D_{hi}}{k_1},$$

where $\bar{S}_1^{lo}$ is the steady state attained with D_{lo} and likewise for $\bar{S}_1^{hi}$. Furthermore, if the difference $D_{hi} - D_{lo}$ is not too big, this oscillation will also not be significantly large.

We will now consider the system (S_2, ρ_2) , where $\rho_2 = \mu_2(S_2)X_2$, and derivate to get $\dot{\rho}_2 = \mu_2 \dot{S}_2 + \mu_2' X_2 \dot{S}_2$:

$$\dot{S}_2 = (S_2^m - S_2) D - k_3 \rho_2 \quad (29)$$

$$\dot{\rho}_2 = \rho_2 \left(\mu_2 - k_{d2} - \alpha D + \frac{\mu_2'}{\mu_2} ((S_2^m - S_2) D - k_3 \rho_2) \right) \quad (30)$$

where

$$S_2^m(t) = S_2^{in} + \frac{k_2}{D} \rho_1(t), \quad (31)$$

and therefore it is also bounded:

$$S_2^{in} + (S_1^m(t) - \bar{S}_1^{lo}) \frac{k_2}{k_1} > S_2^m(t) > S_2^{in} + (S_1^m(t) - \bar{S}_1^{hi}) \frac{k_2}{k_1}.$$

We will analyze the qualitative behavior of the 2D system (29)-(30) by looking at the three nullclines:

$$\rho_2 = N_1(S_2; D) = \frac{D}{k_3} (S_2^m - S_2) \quad (32)$$

$$\rho_2 = N_2(S_2; D) = \frac{D}{k_3} \phi_2(S_2, D) \quad (33)$$

$$\rho_2 = 0 \quad (34)$$

where, after some manipulation of (30):

$$\phi_2(S_2, D) = (S_2^m - S_2) + \frac{\mu_2}{\mu_2'} \left(\frac{\mu_2 - k_{d2} - \alpha D}{D} \right) \quad (35)$$

A steady state is the washout where (32) and (34) intersect, at $\bar{S}_2 = S_2^m$, $\bar{\rho}_2 = 0$. Other steady states might occur where (32) and (33) intersect. When $D = D_{hi}$, $\mu_2(S_2) - k_{d2} - \alpha D_{hi}$ is always negative so N_1 and N_2 do not intersect. When $D = D_{lo}$, $\mu_2(S_2) = k_{d2} + \alpha D_{lo}$ may have two solutions, but only the one where $\bar{S}_2^{lo} < S_2^*$ is stable. Notice that (32) is a line with slope $-D/k_3$, while (33) has an asymptote at S_2^* :

- If $\mu_2^* > k_{d2} + \alpha D$ (the case for D_{lo}), then $\lim_{S_2 \rightarrow S_2^{*-}} \phi_2(S_2; D) = +\infty$, $\lim_{S_2 \rightarrow S_2^{*+}} \phi_2(S_2; D) = -\infty$.

- If $\mu_2^* < k_{d2} + \alpha D$ (the case for D_{hi}), then

$$\lim_{S_2 \rightarrow S_2^{*-}} \phi_2(S_2; D) = -\infty, \quad \lim_{S_2 \rightarrow S_2^{*+}} \phi_2(S_2; D) = +\infty.$$

The phase-space is divided in 4 regions, some of them disconnected and each representing a direction of the vector fields. For the parameters on Table 1, they are shown in Figure 1 for $D_{lo} = 0.379$ (left) and $D_{hi} = 0.547$ (right). The arrows indicate the direction of the vector fields, and the green circle is the stable steady state. The green line corresponds to nullcline (32) and the blue curves to the nullcline (33). Recall that this is the phase plane of an approximate 2D representation of the system; the regions will shift as $S_2^m(t)$ changes within bounds that are ultimately determined by the changes of $X_T^{in}(t)$, $S_1^{in}(t)$ and $S_2^{in}(t)$. However, the qualitative behavior of the trajectories is determined by the direction of the vector fields in the regions, which is unaffected by these changes.

Table 1. Parameters for the (S_2, ρ_2) system.

Parameter	Value	Parameter	Value
μ_2^*	0.45 h ⁻¹	α	0.9
S_2^*	90 mg L ⁻¹	S_2^m	200 mg L ⁻¹
β	0.75	k_{d2}	0.04 h ⁻¹
k_3	1 mg mg ⁻¹		

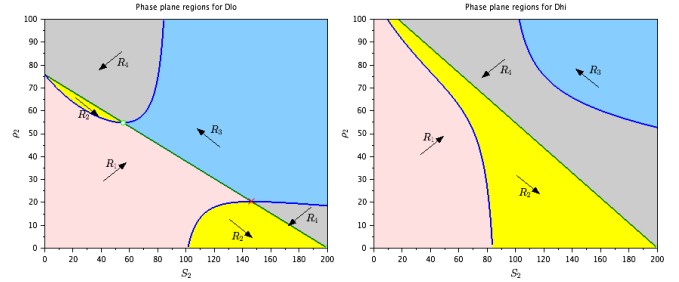


Fig. 1. Phase plane regions for D_{lo} and D_{hi} . Color code: R_1 =pink, R_2 =yellow, R_3 =blue, R_4 =gray.

Figure 2 shows the input/output steady state map. Notice that the maximum rate of ρ_2 is achieved for

$$D_{opt} = 0.421, \quad \bar{S}_2^{opt} = 64.87, \quad \bar{\rho}_2^{opt} = 56.48.$$

Notice that D_{opt} is very close to $D_{cr2} = 0.456$, while $D_{cr1} = 0.288$.

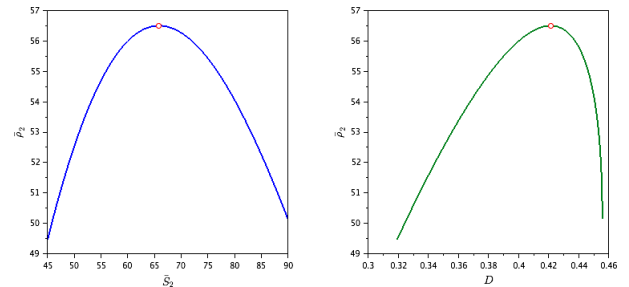


Fig. 2. Steady state input/output maps.

Let us call the regions R_i^{lo} when $D = D_{lo}$ and R_i^{hi} when $D = D_{hi}$, for $i \in \{1, 2, 3, 4\}$. Let $w = (S_2, \rho_2)$ and let $\bar{w}_{lo}$ be the non-washout stable steady state for D_{lo} . Let $w_{lo}(t; w_0)$ and $w_{hi}(t; w_0)$ be the trajectories starting at w_0 when

$D = D_{lo}$ and $D = D_{hi}$, respectively. Suppose that initially $D = D_{lo}$ and w_0 is such that $w(t; w_0) \rightarrow \bar{w}_{lo}$. We follow this trajectory for some time T_1 until $w_1 = w_{lo}(T_1; w_0) \in R_1^{hi}$, close to $\bar{w}_{lo}$. Now we switch to $D = D_{hi}$. The trajectory $w_{hi}(t; w_1)$ will go northeast ($\nearrow$ on R_1^{hi}), cross the curve $\rho_2 = N_2(S_2; D_{hi})$ and then follow a path southeast ($\searrow$ on R_2^{hi}) on its way to the washout of methanogens. We follow this trajectory for some time T_2 so that $w_2 = w_{hi}(T_2; w_1) \in (R_3^{lo} \cup R_1^{lo}) \cap \mathcal{R}_{lo}$. At this point we switch to D_{lo} and the trajectory $w_{lo}(t; w_2)$ will eventually go northwest ($\nwarrow$ on R_3^{lo}), and then cross $\rho_2 = N_2(S_2; D_{lo})$ on its way to $\bar{w}_{lo}$, when it will eventually go south ($\searrow$ on R_4^{lo} , or eventually $\swarrow$ on R_2^{lo}). We follow this trajectory for a time T_3 until $w_3 = w_{lo}(T_3; w_2) \in R_1^{hi}$. We then again change to $D = D_{hi}$ and repeat.

The above discussion implies that by alternating D between D_{lo} and D_{hi} , with adequate times on each condition, the trajectory for $\rho_2(t)$ will reach local maxima periodically. The timely detection of these maxima could be used to oscillate around the maximum achievable value for ρ_2 .

Notice that the condition $\bar{w}_{lo} \in R_1^{hi}$ is met if $\bar{\rho}_2^{lo} < N_2(\bar{S}_2^{lo}; D_{hi})$. Considering that $\mu_2(\bar{S}_2^{lo}) - k_{d2} = \alpha D_{lo}$, using (19), (33), (35) and simplifying,

$$\frac{S_2^m - \bar{S}_2^{lo}}{\alpha} > \frac{\mu_2(\bar{S}_2^{lo})}{\mu_2'(\bar{S}_2^{lo})} = \frac{\frac{\bar{S}_2^{lo}}{S_2^*} + \beta \left(\frac{\bar{S}_2^{lo}}{S_2^*} - 1 \right)^2}{\frac{\beta}{S_2^*} \left(\frac{S_2^*}{\bar{S}_2^{lo}} - \frac{\bar{S}_2^{lo}}{S_2^*} \right)}. \quad (36)$$

It is possible to show that this condition is always satisfied for $\bar{S}_2^{lo}$.

Figure 3 shows the same phase plane for D_{lo} and D_{hi} , but in orange lines the nullclines of the opposite condition are also shown. The steady state $\bar{w}_{lo}$ is shown as a green circle, and the optimum steady state $\bar{w}_{opt}$ is shown as a magenta circle. Notice that $\bar{w}_{lo} \in R_1^{hi}$ as expected.

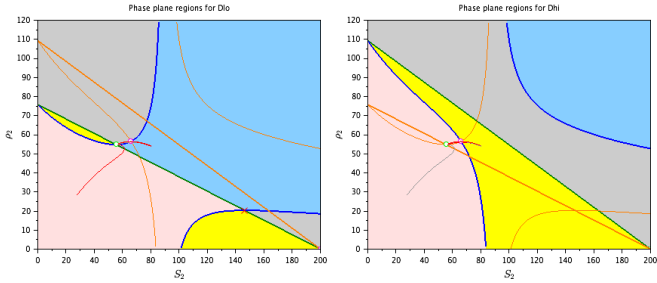


Fig. 3. Trajectories in the phase plane (S_2, ρ_2) for an alternating operation between D_{lo} (left) and D_{hi} (right).

In the figure, shown as a red curve is a trajectory that starts with an initial condition $w_0 \in R_1^{lo}$ and D_{lo} for 10 h, and then alternates between D_{hi} and D_{lo} with $T_{hi} = 1.5$ h and $T_{lo} = 5$ h. Notice that indeed, T_{hi} is such that the trajectory ends in R_3^{hi} , and that T_{lo} is such that the corresponding trajectory ends close to $\bar{w}_{lo}$. It is noticeable that indeed local maxima in $\rho_2(t)$ occur, and they happen very near $\bar{\rho}_2^{opt}$.

The advantage of this qualitative analysis is that it is valid even if S_2^m is (slowly) time-varying, which indeed happens since it depends on $\rho_1(t)$, cf. (31). The nullclines will then “move” as the trajectory evolves; it is to be discussed

how this affects the qualitative analysis. As previously mentioned, for the 2D system (S_1, ρ_1) of (27)–(28), we can follow a similar procedure for its analysis. Consider thus the additional parameters of Table 2.

Table 2. Parameters for the (S_1, ρ_1) system.

Parameter	Value	Parameter	Value
μ_1^*	0.82 h ⁻¹	K_{S1}^*	10 mg L ⁻¹
S_1^m	100 mg L ⁻¹	k_{d1}	0.06 h ⁻¹
k_1	0.8 mg mg ⁻¹	k_2	1.2 mg mg ⁻¹

For the same conditions of transitions between D_{lo} and D_{hi} as above, figure 4 shows the trajectories in red.

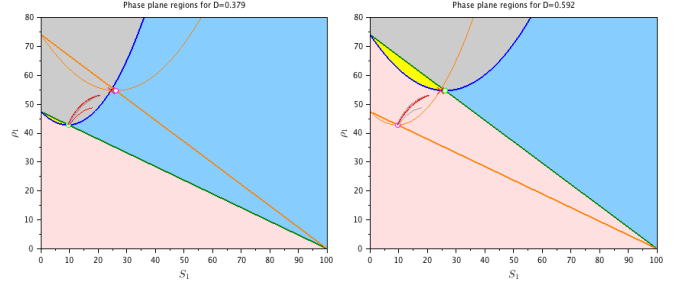


Fig. 4. Trajectories in the phase plane (S_1, ρ_1) for an alternating operation between D_{lo} (left) and D_{hi} (right).

It can be appreciated that $\rho_1(t)$ is bounded between approximately 42.8 and 53.1 mg L⁻¹h⁻¹. Furthermore, $\rho_1(t)$ increases when $D = D_{hi}$, and decreases when $D = D_{lo}$, but since $S_2^m = S_2^{in} + \frac{k_2}{D} \rho_1(t)$, this implies that S_2^m will decrease to values close to $S_2^{in} + 116.5$ when $D = D_{hi}$ and increase to $S_2^{in} + 135.5$ when $D = D_{lo}$. Thus, the trajectory $w_{hi}(t; w_1)$ will start with S_2^m high and end with S_2^m low, implying that the maximum in ρ_2 will be reached faster. On the other hand, since $S_2^m(t)$ increases when $D = D_{lo}$, the trajectory $w_{lo}(t; w_2)$ will start with S_2^m low and end with S_2^m high, risking that the maximum of $\rho_2(t)$ may not be observed.

6. SIMULATIONS

To check that indeed this controller proposal could work, we now simulate the complete system with the same kinetic parameters, but considering the additional parameters on Table 3. In this case, we can find that $D_{cr2} = 0.446$ and $D_{opt} \approx 0.406$. We simulate then first for 10 h with $D_{lo} = 0.3$ and then alternate with $D_{hi} = 0.55$ h⁻¹ for $T_{hi} = 2.5$ h with $D_{lo} = 0.3$ h⁻¹ for $T_{lo} = 5$ h. The results are shown in Figure 5.

Table 3. Additional parameters for simulation.

Parameter	Value	Parameter	Value
k_{hyd}	0.5 h ⁻¹	X_T^{in}	20 mg L ⁻¹
S_1^{in}	85 mg L ⁻¹	S_2^{in}	75 mg L ⁻¹
D_{lo}	0.3 h ⁻¹	D_{hi}	0.55 h ⁻¹

The simulation shows the expected behavior. The third graph (from left to right) of the bottom row shows the evolution of $\rho_2(t)$, which is proportional to the output $q_m(t)$. It is clear that maxima are reached during the

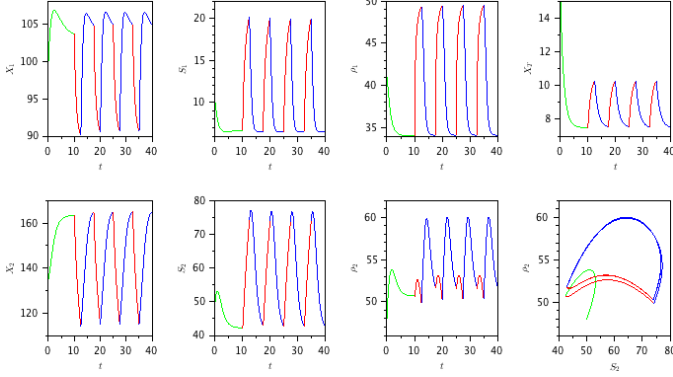


Fig. 5. Simulation of the complete model alternating with $T_{hi} = 2.5$, $D_{hi} = 0.55$ (red) and $T_{lo} = 5$, $D_{lo} = 0.3$ (blue) after an initial period with D_{lo} (green).

transients, both when D changes from D_{lo} to D_{hi} (red curves) and viceversa (blue curves). The fourth graph is the evolution of (S_2, ρ_2) in the state space, showing the occurrence of maxima, too.

However, this behavior does not always happen. For example, if now $S_2^{in} = 25 \text{ mg L}^{-1}$, then $D_{opt} \approx 0.372 \text{ h}^{-1}$ and in fact $\bar{\rho}_2^{opt} \approx 37.88$. Figure 6 shows a simulation alternating with $\bar{D}_{hi} = 0.55 \text{ h}^{-1}$ for $T_{hi} = 1 \text{ h}$ and $D_{lo} = 0.35 \text{ h}^{-1}$ for $T_{lo} = 6 \text{ h}$. Although with D_{lo} we do see the peaks, with D_{hi} we no longer see them. Nevertheless, notice that $\rho_2(t)$ peaks at values even higher than $\bar{\rho}_2^{opt}$.

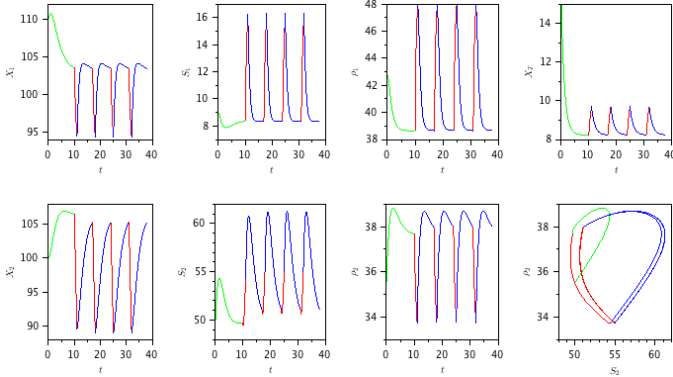


Fig. 6. Simulation of the model alternating with $T_{hi} = 1$, $D_{hi} = 0.55$ (red) and $T_{lo} = 6$, $D_{lo} = 0.6$ (blue) when the VFA influent concentration is decreased.

7. CONCLUSIONS

For an anaerobic bioreactor model, which has proven to be useful in predicting the dynamic behavior of this type of systems, we propose to alternate between two dilution rates to maximize the methane outflow rate. This proposal is based on a detailed qualitative analysis of the transient behavior of the state trajectories, especially that of the measured output. It is shown that indeed, when adequately alternating between dilution rates above and below the optimal steady-state maximizing input, the trajectory of the output signal (the methane flow rate) reaches a temporary maximum. This observation can be used to propose an output feedback maximizing controller, and it is the subject of ongoing research.

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