First Results of Optimal Control of Average Biogas Production for the Chemostat Over an Infinite Horizon

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Abstract: In this work we study the optimal control problem of maximizing the average biogas production over an infinite horizon. We consider a large class of growth rate functions that depend on substrate and biomass concentrations and we solve this problem for the chemostat model. The obtained optimal control is a autonomous state feedback.

Keywords: Optimal Control, Infinite Horizon, Biogas production, Chemostat.

1. INTRODUCTION

Anaerobic digestion is a commonly used process for the biological treatment of wastewater in which organic compounds are decomposed into biogas by a population of microorganisms. The operation of such processes raises a number of challenges, such as the control of operational parameters, since anaerobic digestion is known to be a complex nonlinear and unstable process. As a final product, biogas can be used as a measure of the stability and efficiency and of the process. Moreover, biogas is composed mainly of methane and can thus be used as a renewable energy source, reducing the energetic cost of wastewater treatement. Therefore it is important to find control strategies that maximize biogas production.

Stating this optimal control problem on a finite horizon raises a number of issues. In pratical applications, it can be difficult or even impossible to specify a final time, especially considering that, in general, solutions of finite horizon problems depend on the given time interval and therefore any change mid-course of the planning horizon will result in loss of optimality. For a long time now, researchers working on optimization related to economics have dealt with these difficulties by considering problems over an infinite horizon (Kamien and Schwartz (2012), Seierstad and Sydsaeter (1986)). Such a formulation of optimal control problems also reflects the need for preserving the viability of a system indefinitely.

The problem under consideration in this work has been solved for a finite horizon when the initial condition belongs to a particular one-dimensional invariant manifold, which allows then to write scalar dynamics (Ghouali et al. (2015)). For the general case of any initial condition in the positive orthant, the derivation of the optimal solution is still today an open problem. However, recently a technique which considers a dynamical frame has allowed to propose sub-optimal controllers with explicit bounds on the difference between the optimal value (which is analytically unknown) and the cost of the proposed controllers (Haddon et al. (2017)). As all these controllers (optimal and sub-optimal) conduct the state vector to approach the one-dimensional manifold (as a turnpike, see Rapaport and Cartigny (2004)), one may have the intuition that for an arbitrary large horizon of time, the optimal trajectory has to be very close to this manifold where an optimal controller is known.

With these considerations in mind, we therefore study the maximization of biogas production over an infinite horizon. As the cost is unbounded on a infinite horizon, we have to choose a concept of optimality (Carlson et al. (1991)). The limiting averaged value appears to us the most natural choice in the present context of biotechnology where the process is expected to be operated on a very long duration and the performance expected from the practitioners is to maintain a high average value over time.

We first state the problem of maximizing the average biogas production as an optimal control problem. We then establish general asymptotic properties of the controlled dynamical system and finally we solve the control problem, thereby obtaining a autonomous state feedback.

2. PROBLEM STATEMENT

We consider the following continuous flow stirred tank bioreactor model where a microbial population of concentration x degrades a substrate of concentration s into biomass and biogas :

$$\dot{s} = D(s_{in} - s) - \mu(s, x)x \tag{1}$$

$$\dot{x} = \mu(s, x)x - Dx \tag{2}$$

where s_{in} is the inflow substrate concentration, D is the dilution rate and $\mu(\cdot, \cdot)$ is the specific growth rate. Without any loss of generality we assume that the units of the concentrations s and x are chosen such that the yield conversion factor is equal to one.

We consider here the following class of growth functions that depend on substrate and biomass :

Assumption 1. $(s,x) \mapsto \mu(s,x)$ is a C^2 function defined on $\mathbf{R}_+ \times (\mathbf{R}_+ \setminus \{0\})$ such that, for all $x > 0$

$$\mu(0,x) = 0 \text{ and } \mu(s,x) > 0 \text{ for } s > 0.$$

In addition we assume that $x \mapsto \mu(s,x)$ is non increasing, which models crowding effects, and $x \mapsto \mu(s,x)x$ is non decreasing, which models the fact that having more biomass provides at least the same growth.

Note that this class of functions also contains growth functions that depend only on the substrate concentration.

We consider initial conditions $(s(0), x(0))$ corresponding to the most common operating conditions and denote them

$$\xi = (s_0, x_0) \in \mathcal{D} := [0, s_{in}) \times (0, \infty).$$

It is straightforward to check that $\mathcal{D}$ is invariant by the dynamics (1)-(2).

We seek to maximize biogas production on a infinite horizon by controlling the dilution rate with the constraint $D(t) \in [0, D_{\max}]$, for $t \geqslant 0$, and we now present the precise mathematical formulation of this problem.

2.1 Average biogas production

We define the average biogas production during a time interval $[0,T]$ as

$$J^T(\xi, D(\cdot)) = \frac{1}{T}\int_0^T \mu\big(s(t),x(t)\big)x(t)\,dt$$

and we consider the inferior and superior limits as T goes to infinity :

$$\underline{J}^\infty(\xi, D(\cdot)) = \liminf_{T\to\infty} \frac{1}{T}\int_0^T \mu\big(s(t),x(t)\big)x(t)\,dt \qquad (3)$$

$$\overline{J}^\infty(\xi, D(\cdot)) = \limsup_{T\to\infty} \frac{1}{T}\int_0^T \mu\big(s(t),x(t)\big)x(t)\,dt \qquad (4)$$

The value functions associated to the optimal control problems are then

$$\underline{V}^\infty(\xi) = \sup_{D(\cdot)} \underline{J}^\infty(\xi, D(\cdot)) \qquad (5)$$

$$\overline{V}^\infty(\xi) = \sup_{D(\cdot)} \overline{J}^\infty(\xi, D(\cdot)) \qquad (6)$$

2.2 Counterexample to the existence of the limit

In this section we exhibit a particular control $D(\cdot)$ for which $\underline{J}^\infty(\xi, D(\cdot))$ and $\overline{J}^\infty(\xi, D(\cdot))$, defined in (3) and (4), respectively, do not coincide. For this, let us consider an initial condition $\xi := (\varepsilon, s_{in} - \varepsilon)$ with $\varepsilon \in (0, s_{in})$ fixed. Note that the set $\{x + s = s_{in}\}$ is invariant for dynamics (1)-(2). Consequently, the chosen initial condition ensures that trajectories of (s,x) remains in this set.

For the sake of simplicity, we consider in this section only a substrate dependent growth function although this example also works for more general growth functions.

Consider now the 2 following paths:

(A) Starting at $\xi := (\varepsilon, s_{in} - \varepsilon)$, use the control $D = D_{\max}$ to reach a prescribed level of substrate $s^* \in (\varepsilon, s_{in})$ and of biomass $x^* = s_{in} - s^* > 0$. Then, apply the control $D = 0$ to return to ξ. Denote this control by D_*, and let t_* be the (finite) time necessary to follow this path and I_* be the biogas produced by this path.

(B) Starting at $\xi := (\varepsilon, s_{in} - \varepsilon)$, note that $D = \mu(\varepsilon)$ allows to stay at $(s = \varepsilon, x = s_{in} - \varepsilon)$ for any time interval.

Then, define control $D(\cdot)$ as follows:

- For $t \in [0, t_*]$, set $D = \mu(\varepsilon)$. The biogas production in this period is thus given by $I_\varepsilon := t_*\mu(\varepsilon)(s_{in} - \varepsilon)$.
- For $t \in (2^{2k}t_*, 2^{2k+1}t_*]$, with $k \in \mathbb{N}$, set $D = D_*$ in order to follow the path (A) repeatedly 2^{2k} times. Thus, for each of these intervals the biogas production is given by $2^{2k}I_*$.
- For $t \in (2^{2k+1}t_*, 2^{2k+2}t_*]$, with $k \in \mathbb{N}$, set $D = \mu(\varepsilon)$. Thus, for each of these intervals the biogas production is given by $2^{2k+1}I_\varepsilon$.

So, when we apply control $D(\cdot)$ until a time $2^{2N}t_*$, for a given $N \geqslant 1$, the average biogas production is computed as follows

$$\begin{aligned} K_N &= \frac{1}{2^{2N}t_*}\int_0^{2^{2N}t_*} \mu(s)(s_{in} - s)\,dt \\ &= \frac{1}{2^{2N}t_*}\left(I_\varepsilon + \sum_{k=0}^{N-1} 2^{2k}I_* + \sum_{k=0}^{N-1} 2^{2k+1}I_\varepsilon\right) \\ &= \frac{I_* + 2I_\varepsilon}{t_*}\sum_{j=1}^{N} 2^{-2j} + \frac{I_\varepsilon}{2^{2N}t_*} \end{aligned}$$

which yields

$$K_N \to \frac{I_* + 2I_\varepsilon}{3t_*} =: K_\infty \text{ as } N \to +\infty$$

Here, we have used the fact that the sum $s_N = \sum_{j=1}^N 2^{-2j}$ converges to $1/3$. Indeed, this follows from the next identity:

$$4s_N = \sum_{j=1}^{N} 2^{2(-j+1)} = \sum_{i=0}^{N-1} 2^{-2i} = 1 + s_N - 2^{-2N}$$

However, for the same control $D(\cdot)$, the average biogas production is, up to time $2^{2N+1}t_*$, computed as follows

$$\begin{aligned} L_N &= \frac{1}{2^{2N+1}t_*}\int_0^{2^{2N+1}t_*} \mu(s)(s_{in} - s)\,dt \\ &= \frac{1}{2^{2N+1}t_*}\left(2^{2N}t_*K_N + 2^{2N}I_*\right) \\ &= \frac{1}{2}\left(K_N + \frac{I_*}{t_*}\right) \end{aligned}$$

which yields

$$L_N \to \frac{2I_* + I_\varepsilon}{3t_*} =: L_\infty \text{ as } N \to +\infty$$

Hence, since $s_* > \varepsilon$ it follows that $I_* > I_\varepsilon$, and consequently, $L_\infty > K_\infty$. We thus obtain that

$$\overline{J}^\infty(\xi, D(\cdot)) \geq L_\infty > K_\infty \geq \underline{J}^\infty(\xi, D(\cdot))$$

3. PRELIMINARY RESULTS

In this section we prove results on the trajectories of (1)-(2) and their associated rewards. For this, we introduce the change of variables, on $\mathcal{D}$,

$$z = \frac{x}{s_{in} - s}$$

and denoting $\zeta = (s, z)'$ the dynamics become

$$\dot{\zeta} = f(\zeta, D) = \begin{pmatrix} \left[D - \mu\big(s, (s_{in} - s)z\big)z\right](s_{in} - s) \\ \mu\big(s, (s_{in} - s)z\big)(1 - z)z \end{pmatrix} \quad (7)$$

Defining

$$\phi(s, z) = \mu\big(s, (s_{in} - s)z\big)(s_{in} - s)$$

and denoting initial conditions again as $\xi = (s_0, z_0)'$, the average reward (3) becomes

$$\underline{J}^\infty(\xi, D(\cdot)) = \liminf_{T\to\infty} \frac{1}{T} \int_0^T \phi\big(s(t), z(t)\big) z(t)\, dt$$

and similarly for the reward (4).

We have the following general property of the controlled dynamical system :

Lemma 2. For a given initial condition $\xi \in \mathcal{D}$ the set

$$\mathcal{L}(\xi) = [0, s_{in}] \times [\min(z_0, 1), \max(z_0, 1)]$$

is an invariant compact set for the system (7), for all admissible controls.

Proof. From Assumption 1 we have that $\mu(\cdot,\cdot) \geqslant 0$ and since the solutions $z(\cdot)$ satisfy (7), we clearly have the following :

$$\min(z_0, 1) \leqslant z(t) \leqslant \max(z_0, 1)$$

for all $t \geqslant 0$, for all admissible controls. $\square$

We now establish a important asymptotic property of the controlled dynamical system by considering only *exciting* controls, that is controls such that

$$\int_0^T D(t)\, dt \underset{T\to\infty}{\longrightarrow} \infty$$

This does not rule out the optimal controls as we only exclude the trajectories where $s(t)$ converges to 0 for which the biogas production also goes to 0.

Lemma 3. For all initial conditions and for all admissible exciting controls, $z(t)$ converges to 1 and

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t z(t)\, dt = 1$$

Proof. As we have seen, with the considered controls, $s(t)$ remains positive for all $t \geqslant 0$, so the convergence of $z(t)$ then follows from (7). Thus for all $\varepsilon > 0$, there exits a time t_ε such that, for all $t \geqslant t_\varepsilon$,

$$|z(t) - 1| < \varepsilon$$

Therefore, for all $T \geqslant t_\varepsilon^2$

$$\begin{aligned} \left|\frac{1}{T}\int_0^T z(t)\, dt - 1\right| &= \frac{1}{T}\left|\int_0^{t_\varepsilon} z(t) - 1\, dt + \int_{t_\varepsilon}^T z(t) - 1\, dt\right| \\ &< \frac{t_\varepsilon}{T}\big(\max(z_0, 1) - 1\big) + \frac{T - t_\varepsilon}{T}\varepsilon \\ &< \frac{z_0}{t_\varepsilon} + \left(1 - \frac{1}{t_\varepsilon}\right)\varepsilon \end{aligned}$$

and we get the desired result since t_ε goes to ∞ as ε goes to 0. $\square$

We now show that both average rewards are well defined.

Lemma 4. For all initial conditions and for all admissible controls the rewards $\underline{J}^\infty(\xi, D(\cdot))$ and $\overline{J}^\infty(\xi, D(\cdot))$ are finite.

Proof. This follows from the fact that there exists a compact invariant set for each initial condition (Lemma 2) and therefore $\phi\big(s(t), z(t)\big)z(t)$ is upper bounded by some constant M_ϕ for all $t \geqslant 0$. Thus $\underline{J}^\infty(\xi, D(\cdot)) \leqslant M_\phi$ and $\overline{J}^\infty(\xi, D(\cdot)) \leqslant M_\phi$. $\square$

4. RESOLUTION OF OPTIMAL CONTROL PROBLEMS

We first give a upper bound of $\overline{V}^\infty(\xi)$. For this, we need the following assumption :

Assumption 5. The function

$$s \mapsto \phi(s, 1) = \mu(s, s_{in} - s)(s_{in} - s)$$

admits a unique maximum $\bar{s}$ on $[0, s_{in}]$.

Note that the Monod function

$$\mu_M(s) = \frac{\mu_{\max} s}{K_s + s}$$

the Haldane function

$$\mu_H(s) = \frac{\bar{\mu} s}{K_s + s + \frac{s^2}{K_i}}$$

and the Contois function

$$\mu_C(s, x) = \frac{\mu_{\max} s}{Kx + s}$$

fullfill Assumptions 1 and 5, for all $\mu_{\max} \in \mathbf{R}_+$, $\bar{\mu} \in \mathbf{R}_+$, $K_s \in \mathbf{R}_+$, $K \in \mathbf{R}_+$, and $K_i \in \mathbf{R}_+$. Indeed, these functions clearly satisfy Assumption 1 and for Assumption 5 see Haddon et al. (2017).

Proposition 6. Under assumption 5, for all initial conditions

$$\overline{V}^\infty(\xi) \leqslant \phi(\bar{s}, 1)$$

Proof. With the assumptions we made on $\mu(\cdot,\cdot)$, we have that $z \mapsto \phi(s, z)$ is non increasing and $z \mapsto \phi(s, z)z$ is inscreasing. This implies that

$$\begin{aligned} \phi(s, \min(z_0, 1)) \min(z_0, 1) &\leqslant \phi(s, z)z \\ &\leqslant \phi(s, \max(z_0, 1)) \max(z_0, 1) \end{aligned} \quad (8)$$

and

$$\phi(s, \max(z_0, 1)) \leqslant \phi(s, z) \leqslant \phi(s, \min(z_0, 1)) \quad (9)$$

Thus, for any control $D(\cdot)$ and for $z_0 \leqslant 1$ we have

$$\begin{aligned} J^T(\xi, D(\cdot)) &\leqslant \frac{1}{T}\int_0^T \phi\big(s(t), \max(z_0, 1)\big) \max(z_0, 1)\, dt \\ &\leqslant \phi(\bar{s}, 1). \end{aligned}$$

Taking the (upper) limit as T goes to ∞ and the supremum in $D(\cdot)$ we get the result. For $z_0 \geqslant 1$ we have

$$\begin{aligned} J^T(\xi, D(\cdot)) &\leqslant \frac{1}{T}\int_0^T \phi\big(s(t), \min(z_0, 1)\big) z(t)\, dt \\ &\leqslant \phi(\bar{s}, 1) \frac{1}{T}\int_0^T z(t)\, dt. \end{aligned}$$

Using Lemma 3 we get that $\overline{J}^\infty(\xi, D(\cdot)) \leqslant \phi(\bar{s}, 1)$ and again we can conclude taking the supremum in $D(\cdot)$. $\square$

This propostion means that the value functions are upper bounded by the biogas flow rate $\phi(s, z)z$ at $s = \bar{s}$ and $z = 1$. With Lemma 3 we already know that an optimal control makes z converge to 1, so we need a control which insures that s reaches $\bar{s}$ to show that the value functions coincide with $\phi(\bar{s}, 1)$.

Definition 7. We define the *most rapid approach control* to $\bar{s}$ as the following feedback

$$\psi_{\bar{s}}(s,z) = \begin{cases} 0 & \text{if } s > \bar{s} \\ \mu(\bar{s},(s_{in}-\bar{s})z)z & \text{if } s = \bar{s} \\ D_{\max} & \text{if } s < \bar{s} \end{cases}. \tag{10}$$

For this feedback to be admissible we need to make the following assumption

Assumption 8. The upper bound on the controls is such that

$$D_{\max} > \mu\big(\bar{s},(s_{in}-\bar{s})\max(z_0,1)\big)\max(z_0,1)$$

This condition also insures that $\bar{s}$ is reachable in finite time with the feedback $\psi_{\bar{s}}$. Indeed, if $s(t) < \bar{s}$ then

$$\dot{s}(t) = \big[D_{\max} - \mu\big(s,(s_{in}-s)z\big)z\big]\,(s_{in}-s) > 0$$

Note that for $s(t) > \bar{s}$, then

$$\dot{s}(t) = -\mu\big(s,(s_{in}-s)z\big)z(s_{in}-s) < 0$$

so that $\bar{s}$ is always reachable.

Proposition 9. For all initial conditions in $\xi \in \mathcal{D}$ we have

$$\phi(\bar{s},1) \leqslant \underline{J}^{\infty}(\xi,\psi_{\bar{s}}) = \overline{J}^{\infty}(\xi,\psi_{\bar{s}})$$

Thus $\psi_{\bar{s}}$ is optimal for both average production problems and we have

$$\underline{V}^{\infty}(\xi) = \overline{V}^{\infty}(\xi) = \phi(\bar{s},1)$$

Proof. We start by pointing out that for the solutions associated to the feedback $\psi_{\bar{s}}$ we have $t_1 = \inf\{t \geqslant 0 : s(t) = \bar{s}\} < \infty$ since $\bar{s}$ is reachable in finite time when Assumption 8 is verified.

If $z_0 \leqslant 1$ we have, for $T > t_1$, using (9)

$$\begin{aligned} J^T(\xi,\psi_{\bar{s}}) &= \frac{1}{T}\Bigg(\int_0^{t_1} \phi(s(t),z(t))z(t)\,dt \\ &\qquad + \int_{t_1}^{T} \phi(\bar{s},z(t))z(t)\,dt\Bigg) \\ &\geqslant \frac{1}{T}\Bigg(\int_0^{t_1} \phi(s(t),z(t))z(t)\,dt \\ &\qquad + \phi(\bar{s},1)\int_{t_1}^{T} z(t)\,dt\Bigg) \end{aligned}$$

and taking the limit as T goes to infinity we get the desired result.

If $z_0 \geqslant 1$ we have, for $T > t_1$, using (8)

$$\begin{aligned} J^T(\xi,\psi_{\bar{s}}) \geqslant \frac{1}{T}\Bigg(&\int_0^{t_1} \phi(s(t),z(t))z(t)\,dt \\ &+ \phi(\bar{s},1)(T-t_1)\Bigg) \end{aligned}$$

and we conclude by taking the limit as T goes to infinity. Notice that here the limit of $J^T(\xi,\psi_{\bar{s}})$ exits, so that we have $\underline{J}^{\infty}(\xi,\psi_{\bar{s}}) = \overline{J}^{\infty}(\xi,\psi_{\bar{s}})$. The optimality of $\psi_{\bar{s}}$ then follows from Proposition 6. □

Remark 10. It is known that the proposed feedback $\psi_{\bar{s}}$ is not optimal for a finite horizon but it is however possible to estimate the suboptimality of this control as it is shown in Haddon et al. (2017).

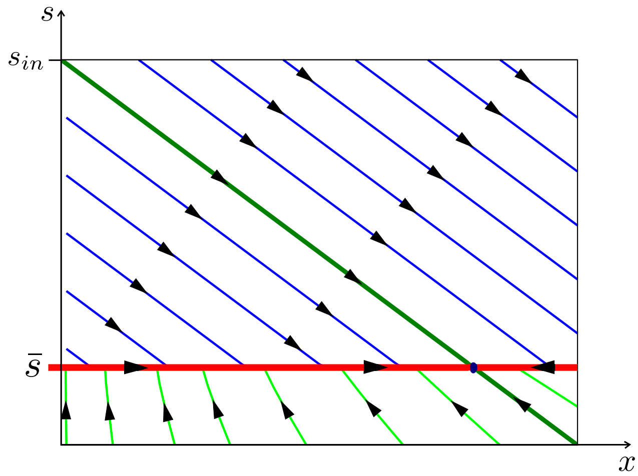

Fig. 1. Optimal synthesis for Haldane growth function

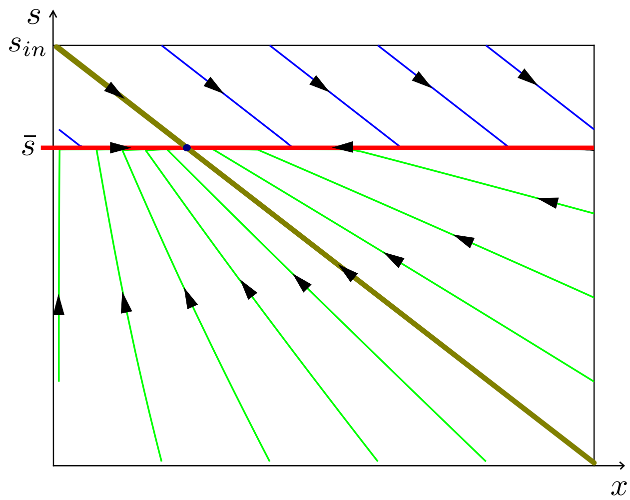

Fig. 2. Optimal synthesis for Contois growth function

We illustrate the feedback $\psi_{\bar{s}}$ by plotting the associated trajectories in state space, in Figure 1 for a Haldane growth function and in Figure 2 for a Contois growth function. The trajectories for a Monod growth function are similar to those for a Haldane growth function, indeed a Monod function can be seen as a Haldane function with very large K_i.

In Figures 3 and 4 we show the open loop realization of the feedback $\psi_{\bar{s}}$ along with the substrate and biomass concentrations as well as the biogas flowrate.

Finally, Figure 5 shows the convergence of the average biogas production to $\phi(\bar{s},1)$ for a Contois growth function, for initial conditions with various different s_0.

5. CONCLUSION

In this work, we have solved the optimal control problem of maximizing the average biogas production over a infinite horizon for the classical model of the chemostat. The optimal control is obtained in autonomous state feedback form which has advantages in terms of robustness.

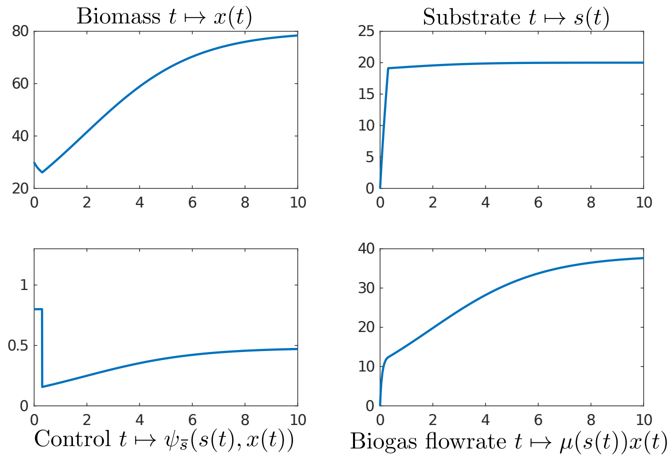

Fig. 3. Time evolution of substrate and biomass concentrations, optimal control and biogas flowrate for a Haldane growth function and for $s_0 < \bar{s}$.

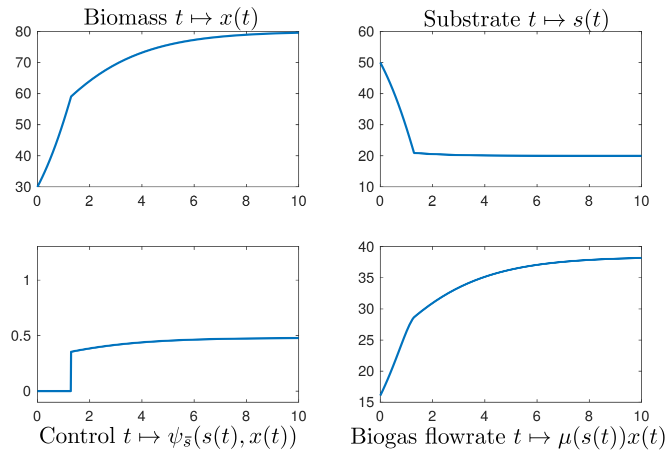

Fig. 4. Time evolution of substrate and biomass concentrations, optimal control and biogas flowrate for a Haldane growth function and for $s_0 > \bar{s}$.

In the (s, x) variables the optimal feedback has the following form :

$$\psi_{\bar{s}}(s,x) = \begin{cases} 0 & \text{if } s > \bar{s} \\ \dfrac{\mu(\bar{s},x)x}{s_{in} - s} & \text{if } s = \bar{s} \\ D_{\max} & \text{if } s < \bar{s} \end{cases}$$

Substrate measurements are necessary for the implementation of this feedback. For the computation of the control when $s = \bar{s}$, biomass measurements could be used but there are alternative solutions : one possibility is to use the biogas flow rate since it is proportional to $\mu(s, x)x$.

In pratice, it can be difficult to set the effective dilution rate on a continuous range of intervals (i.e. only a discrete set of values are possible) and changes of rate usually can only happen at discrete instants, according to the frequncy of the actuators. In this situtation, one can use chattering to maintain the substrate level at $\bar{s}$, see Zelikin and Borisov (2012).

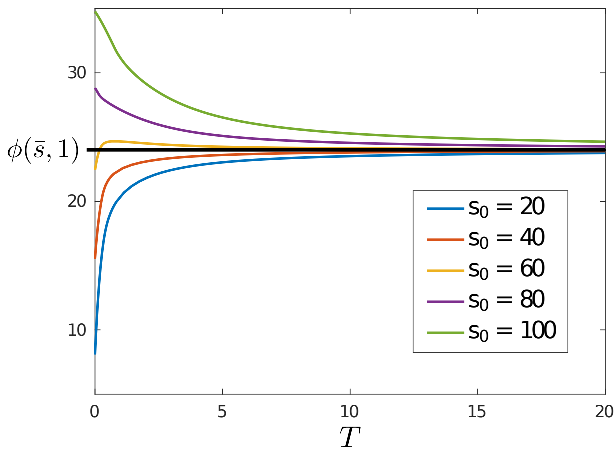

Fig. 5. Average biogas production $T \mapsto J^T(\xi, \psi_{\bar{s}})$, for different initial substrate concentrations, with a initial biomass concentration of $x_0 = 50$ and for a Contois growth function. The black line represents the value functions $\underline{V}^{\infty}(\xi) = \overline{V}^{\infty}(\xi) = \phi(\bar{s}, 1)$ that are constant for all initial conditions in $\mathcal{D}$.

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