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 Guaranteed value strategy for the optimal control of biogas production in continuous bio-reactors

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Abstract: In this work, we revisit a problem of optimal control for the maximisation of biogas production in a continuous bioreactor, for which the analytical determination of the optimal synthesis is an open problem. We consider two kinds of growth rates: substrate dependent or substrate and biomass dependent. We propose a sub-optimal controller, as a most rapid approach path strategy, and moreover we provide guaranteed bounds for the unknown value function of the optimal control problem. This controller has the property of being a stationary state feedback for the substrate dependent case, even though the optimal control problem is with fixed finite terminal time.

Keywords: optimal control, value function, sub-optimal controller, bioreactor.

1. INTRODUCTION

Anaerobic digestion is a complex biological process which is used in wastewater treatment to remove organic compounds from water. In this process, organic compounds are transformed into biogas (mainly composed of carbon dioxide and methane) by different microbial populations and this biogas can be used as an energy source, thereby reducing the energetic cost of wastewater treatment. Among the different challenges raised by the industrial application of this technology is the control of the operational parameters to guarantee process stability and performance. As biogas is a final product it can be used as a measure of the efficiency and stability of the anaerobic digestion and therefore, there is a strong interest in finding optimal control strategies that maximize biogas production.

Many studies have been conducted on the control of anaerobic digestion and there exists various different strategies that can be divided in 2 categories: model based and knowledge based. The latter are mainly proposed by experts of anaerobic digestion (such as bioprocess engineers) who construct strategies based on practical knowledge. They generally focus on process stability although there are studies that aim to maximize performance such as Steyer et al. (1999) and Rodriguez et al. (2006). On the other hand, model based controllers are developed by the automatic control community and the main advantage of this approach is the theoretical properties that they can guarantee such as robustness or performance, see Bonnans and Rouchon (2005) and Bressan and Piccoli (2007). One of the first attempts at using the theory of optimal control for the problem of maximizing the methane production over a given time interval was done by Stamatelatou et al. (1997). Here a single step model is used and by applying the Pontryagin maximum principle the singular arcs are computed, however there is no synthesis of the optimal control. This problem is also studied in Ghouali et al. (2015) where the model is reduced to a single equation by taking particular initial conditions lying on a 1d subset and the full optimal synthesis is given.

In this work, we study the problem of maximizing the methane production with the full single step model: at this time, the analytic resolution of this optimal control problem is open. An analytic determination of the optimal state feedback would be very valuable for practitioners as it is easy and robust to apply. Nevertheless, we propose instead a guaranteed value strategy with a suboptimal feedback control law for two kinds of growth rate: substrate dependant (such as Monod) or substrate and biomass dependant (such as Contois). Using an auxiliary control problem, we establish a guaranteed frame for the value function of the main problem and we then prove that this strategy is optimal for the auxiliary problem. Furthermore, the feedback we propose is autonomous when the growth rate is not density dependent and this has robustness advantages for applications in terms of possible time delays of the control as well as changes of the final time during process operation.
2. MODEL DESCRIPTION AND CONTROL PROBLEMS

Consider the following dynamics which model a continuously fed bioreactor where a substrate of concentration \( s \) is degraded by a microbial population of concentration \( x \) into biomass and biogas controlled by the dilution rate \( u \) which is the controlled variable:

\[
\begin{align*}
\dot{s} &= -\mu(s)x + u(s_{in} - s) \\
\dot{x} &= \mu(s)x - ux
\end{align*}
\]

where \( s_{in} \) is the input concentration and \( \mu(\cdot) \) is the specific growth rate. We consider two kinds of growth functions \( \mu(\cdot) \):

- substrate dependent (SD type): \( C^2 \) functions \( s \mapsto \mu(s) \) defined in \( \mathbb{R}_+ \) such that
  
  \[
  \mu(0) = 0 \quad \text{and} \quad \mu(s) > 0 \quad \text{for} \quad s > 0.
  \]

- substrate and biomass dependent (SBD type): \( C^2 \) functions \( (s, z) \mapsto \mu(s, z) \) defined on \( \mathbb{R}_+ \times (\mathbb{R}_+ \setminus \{0\}) \) such that for any \( x > 0 \) one has
  
  \[
  \mu(0, x) = 0 \quad \text{and} \quad \mu(s, x) > 0 \quad \text{for} \quad s > 0.
  \]

Moreover we shall assume that \( x \mapsto \mu(s, x) \) is non increasing and \( x \mapsto \mu(s, x) \) is increasing.

We consider initial conditions and control bounds corresponding to the most common operating conditions:

\[
(s(0), x(0)) = (s_0, x_0) \in [0, s_{in}) \times [0, +\infty)
\]

and

\[
u(t) \in [0, u_{\text{max}}], \quad \forall t \in [0, T].
\]

The optimal control problem studied here is the maximisation of the following cost, that represents the cumulated biogas extracted from the bioreactor, independently from the control, between initial and terminal times. For the SD case:

\[
J(t_0, s_0, x_0, u(\cdot)) = \int_{t_0}^{T} \mu(s(t))x(t) \, dt
\]

and for the SBD case:

\[
J_{SB}(t_0, s_0, x_0, u(\cdot)) = \int_{t_0}^{T} \mu(s(t), x(t))x(t) \, dt
\]

As one has \( s(t) < s_{in} \) for any \( t \geq 0 \) and any control law \( u(\cdot) \), one can consider the change of coordinates

\[
\begin{pmatrix} s \\ z \end{pmatrix} \rightarrow \begin{pmatrix} s \\ z \end{pmatrix} \quad \text{with} \quad z = \frac{x}{s_{in} - s}.
\]

One can straightforwardly check that the dynamics in \((s, z)\) coordinates is

\[
\begin{align*}
\dot{s} &= (s_{in} - s)(-\mu(\cdot)z + u) \\
\dot{z} &= \mu(\cdot)z(1 - z)
\end{align*}
\]

The cost for the SD case is

\[
J(t_0, s_0, z_0, u(\cdot)) = \int_{t_0}^{T} \phi(s(t))z(t) \, dt
\]

where the function \( \phi(\cdot) \) is defined as

\[
\phi(s) = \mu(s)(s_{in} - s).
\]

The cost in the SBD case is

\[
J_{SB}(t_0, s_0, z_0, u(\cdot)) = \int_{t_0}^{T} \phi_{SB}(s(t), z(t))z(t) \, dt
\]

where the function \( \phi_{SB}(\cdot, \cdot) \) is defined as

\[
\phi_{SB}(s, z) = \mu(s, s_{in} - s)z(s_{in} - s).
\]

We finish this section with the following definition:

**Definition 1.** We define as admissible feedback for an initial condition \((s_0, z_0)\) a function \( (s, z) \mapsto \psi(s, z) \) such that the solution \((s(\cdot), z(\cdot))\) with \( u = \psi(s, z) \) satisfies \( \psi(s, z) \in [0, u_{\text{max}}] \) for all \( t \in [0, T] \).

3. GUARANTEED COST VALUE : SUBSTRATE DEPENDENT

We consider the auxiliary optimal control problem for the criterion

\[
J(t_0, s_0, z_0, u(\cdot)) = \int_{t_0}^{T} \phi(s(t)) \, dt
\]

instead of \( J(\cdot) \). Denote \( V(\cdot) \) and \( W(\cdot) \) the value functions associated, respectively, to the original and the auxiliary problem:

\[
V(t_0, s_0, z_0) = \max_{u(\cdot)} J(t_0, s_0, z_0, u(\cdot)),
\]

\[
W(t_0, s_0, z_0) = \max_{u(\cdot)} \tilde{J}(t_0, s_0, z_0, u(\cdot)).
\]

Clearly, one has, for all \( t \in [0, T] \):

\[
\min(z_0, 1) \leq z(t) \leq \max(z_0, 1)
\]

for any solution \( z(\cdot) \), whatever is the control \( u(\cdot) \). Then one has the following frame for the function \( V(\cdot) \):

\[
\min(z_0, 1)W(t_0, s_0, z_0) \leq V(t_0, s_0, z_0) \leq \max(z_0, 1)W(t_0, s_0, z_0).
\]

Moreover, any optimal control \( \tilde{u}^*(\cdot) \) for the cost \( \tilde{J} \) guarantees a (sub-optimal) value for the criterion \( J \) that fulfills

\[
\min(z_0, 1)W(t_0, s_0, z_0) \leq J(t_0, s_0, z_0, \tilde{u}^*(\cdot)) \leq \max(z_0, 1)W(t_0, s_0, z_0).
\]

4. GUARANTEED COST VALUE : SUBSTRATE AND BIOMASS DEPENDENT

We now consider the following auxiliary optimal control problems for the criterions

\[
\tilde{J}_{SB}(t_0, s_0, z_0, u(\cdot)) = \int_{t_0}^{T} \phi_{SB}(s(t), \min(1, z_0)) \, dt
\]

\[
\tilde{J}_{SB}(t_0, s_0, z_0, u(\cdot)) = \int_{t_0}^{T} \phi_{SB}(s(t), \max(1, z_0)) \, dt
\]
instead of $J_{SB}(\cdot)$. Denote $V_{SB}(\cdot), \tilde{W}_{SB}(\cdot)$ and $\hat{W}_{SB}(\cdot)$ the value functions associated, respectively, to the original and the auxiliary problems:
\begin{align}
V_{SB}(t_0, s_0, z_0) &= \max_{u(\cdot)} J_{SB}(t_0, s_0, z_0, u(\cdot)), \\
\tilde{W}_{SB}(t_0, s_0, z_0) &= \max_{u(\cdot)} \tilde{J}_{SB}(t_0, s_0, z_0, u(\cdot)) \\
\hat{W}_{SB}(t_0, s_0, z_0) &= \max_{u(\cdot)} \hat{J}_{SB}(t_0, s_0, z_0, u(\cdot)).
\end{align}

Since $z \mapsto \phi_{SB}(s, z)$ is increasing we have
\[
\phi_{SB}(s, \min(z_0, 1)) \min(z_0, 1) \leq \phi_{SB}(s, z) z \\
\leq \phi_{SB}(s, \max(z_0, 1)) \max(z_0, 1).
\]

From these inequalities we can establish two frames for the $x$ function
\[
J \leq \mu(s, x) \leq J \mu(s, x) = \mu(s, x).
\]

Moreover, any optimal control $\hat{u}^*(\cdot)$ for the cost $\tilde{J}_{SB}$ fulfills
\[
\min(z_0, 1)\tilde{W}_{SB}(t_0, s_0, z_0) \leq \tilde{J}_{SB}(t_0, s_0, z_0, \hat{u}^*(\cdot)) \\
\leq \max(z_0, 1)W_{SB}(t_0, s_0, z_0).
\]

Secondly, we also have
\[
\min(z_0, 1)\tilde{W}_{SB}(t_0, s_0, z_0) \leq V_{SB}(t_0, s_0, z_0) \\
\leq \max(z_0, 1)W_{SB}(t_0, s_0, z_0).
\]

We make the following assumption on the function $\gamma(\cdot)$:

**Assumption 3.** The function $s \mapsto \gamma(s)$ is non-negative with $\gamma(0) = \gamma(s_{in}) = 0$ and admits a unique maximum $\bar{s}$ on $[0,s_{in}]$.

This assumption is indeed verified for the usual growth function as the following result show :

**Lemma 4.** For all $\mu_{\text{max}} \in \mathbb{R}_+, K \in \mathbb{R}_+, K_i \in \mathbb{R}_+$ the Monod function
\[
\mu_M(s) = \frac{\mu_{\text{max}}s}{K + s}
\]

fulfills the previous assumption.

**Proof.** Let us first show that the function $\mu_M$ is increasing and strictly concave:
\[
\mu_M'(s) = \frac{\mu_{\text{max}}K}{(K + s)^2} > 0, \quad \mu_M''(s) = -2\frac{\mu_{\text{max}}K}{(K + s)^3} < 0.
\]

Notice that the function $\phi$ is non-negative on $[0,s_{in}]$ with $\phi(0) = \phi(s_{in}) = 0$. Therefore it admits a maximum on $[0,s_{in}]$. One has
\[
\phi'(s) = \mu_M'(s)(s_{in} - s) - \mu_M(s) \\
\phi''(s) = \mu_M''(s)(s_{in} - s) - 2\mu_M'(s)
\]

The function $\phi$ is thus strictly concave on $[0,s_{in}]$, which provides the uniqueness of its maximum.

For the Haldane function, we have:
\[
\phi'(s) = \mu_{\text{max}} \frac{s_{in}K - 2Ks + s^2(1 + \frac{s_{in}}{K_2})}{(K + s + \frac{s^2}{K_2})^2}
\]
such that $\phi'(0) > 0$ and $\phi'(s_{in}) < 0$ and since $\phi'$ is continuous it must have an odd number of zeroes in the interval $[0,s_{in}]$. But notice that the equation $\phi'(s) = 0$ admits at most 2 solutions and $\phi(0) = \phi(s_{in}) = 0$ and therefore $\phi$ has a unique maximum.

For the Contois function, notice that $\mu_C(s, x) = \mu_M(s/x)$ so that
\[
\phi_{SB}(s, \min(z_0, 1)) = \mu_M \left( \frac{s_{in}}{(s_{in} - s) \min(z_0, 1)} \right) (s_{in} - s)
\]
and since $s \mapsto \frac{s_{in} - s}{(s_{in} - s) \min(z_0, 1)}$ is an increasing function, $\phi_{SB}(\cdot, \min(z_0, 1))$ is also strictly concave and the same argument is valid for $\phi_{SB}(\cdot, \max(z_0, 1))$.

**Remark 5.** For the SD case $\bar{s}$ is independent of $z_0$, while for the SBD case it does depend on the initial value $z_0$.

We define the most rapid approach feedback to $s = \bar{s}$, as
\[
\psi_{\bar{s}}(s, z) = \begin{cases} 
0 & \text{if } s > \bar{s} \\
\mu_{\text{max}} & \text{if } s = \bar{s} \\
\hat{u}_{\text{max}} & \text{if } s < \bar{s}
\end{cases}
\]
In particular for the SD case we have $\mu(\cdot)|_{s=\bar{s}} = \mu(\bar{s})$ and for the SBD case we have $\mu(\cdot)|_{s=\bar{s}} = \mu(\bar{s}, (s_{in} - \bar{s}) z)$.

**Remark 6.** This feedback is admissible, in the SD case, if $\max(1, z_0) \mu(\cdot) \leq u_{\max}$. In the SBD case, it is admissible for problem (13) if

$$\phi_{SB}(\bar{s}, \min(z_0, 1)) \max(1, z_0) \leq u_{\max}$$

and for problem (14) if

$$\phi_{SB}(\bar{s}, \max(z_0, 1)) \max(1, z_0) \leq u_{\max}$$

**Remark 7.** Note that, in the SD case, this feedback coincides with the optimal feedback of Ghouali et al. (2015) for the particular initial conditions such that $z_0 = 1$, which is an invariant.

**Remark 8.** In the SD case, $\phi$ being independent of $z_0$, the feedback does not depend on the initial condition: it is an autonomous state feedback (while the problem is with finite horizon). For the SBD case the feedback does depend on the initial value of $z_0$ : the feedback is not autonomous in this case.

**Remark 9.** For the implementation of this feedback measurements of the substrate are necessary. In addition, an estimation of

$$\mu(\cdot) z = \frac{\mu(\cdot) x}{s_{in} - s}$$

is needed to compute the value of the control when $s = \bar{s}$. This can be achieved using biomass measurements but there are several other possibilities: one solution is to use the biogas flow rate as it is proportional to $\mu(\cdot) x$; another solution is to use chopping to maintain the substrate close to the optimal level, see Zelikin and Borisov (2012).

**Proposition 10.** The feedback (18) is optimal for the auxiliary problem (17), for any initial condition such that (18) is admissible.

**Proof.** We denote by $s(t, t_0, s_0, z_0, u)$ the solution associated to the control $u$, at time $t$ with initial conditions $(s(t_0), z(t_0)) = (s_0, z_0)$. We start with $s_0 \geq \bar{s}$. Then we have

$$\dot{s}(t, t_0, s_0, 0) = -\mu(\cdot)(s_{in} - s) \leq 0$$

and therefore there exists a time $t_{\min}$, possibly larger than $T$, such that $s(t_{\min}) = \bar{s}$. Thus the solution associated to the feedback (18) is, with $t_* = \min(t_{\min}, T)$:

$$s(t, t_0, s_0, 0, \psi_s) = \begin{cases} s(t, t_0, s_0, 0) & \text{if } t < t_* \\ \bar{s} & \text{if } t_* \leq t \leq T \end{cases}$$

In this case, for any value $u \in [0, u_{\max}]$ and for any values $(s, z) \in (\bar{s}, s_{in}) \times (0, u_{\max}/\mu(\bar{s}))$ :

$$-\mu(\cdot)(s_{in} - s)z \leq (s_{in} - s)u - \mu(\cdot)(s_{in} - s)z$$

and thus denoting $f(s, z, u)$ the right hand side of (5) we have $f(s, z, 0) \leq f(s, z, u)$. By the theorem of comparison of dynamical systems, this implies that $s(t_0, t_0, s_0, 0) \leq s(t, t_0, s_0, 0, u)$, up to time $t_*$. Since $\gamma$ is decreasing on $[\bar{s}, s_{in}]$, we have for any admissible control $u$:

$$\gamma(s(t, t_0, s_0, 0)) \geq \gamma(s(t, t_0, s_0, 0, u))$$

Finally, since $\gamma$ reaches its maximum at $\bar{s}$ we get

$$K(t_0, s_0, z_0, \psi_s) = \int_{t_0}^{t_*} \gamma(s(t, t_0, s_0, 0)) dt + \int_{t_*}^{T} \gamma(\bar{s}) dt$$

$$\geq \int_{t_0}^{t_*} \gamma(s(t, t_0, s_0, 0, u)) dt$$

$$= K(t_0, s_0, z_0, u)$$

We now consider $s_0 < \bar{s}$. Since the feedback is admissible we have that

$$u_{\max} \geq \mu(\cdot) z$$

Thus, we have

$$s(t, t_0, s_0, u_{\max}) = (s_{in} - s)(-\mu(\cdot) z + u_{\max}) \geq 0$$

and therefore there exists a time $t_{\max}$, possibly larger than $T$, such that $s(t_{\max}) = \bar{s}$. Thus the solution associated to the feedback (18) is, with $t_* = \min(t_{\max}, T)$ :

$$s(t, t_0, s_0, 0) = \begin{cases} s(t, t_0, s_0, 0, u_{\max}) & \text{if } t_0 < t < t_* \\ \bar{s} & \text{if } t_* \leq t \leq T \end{cases}$$

In this case, for any value $u \in [0, u_{\max}]$ and for any values $(s, z) \in (\bar{s}, \bar{s}) \times (0, u_{\max}/\mu(\bar{s}))$ :

$$(s_{in} - s)(u - \mu(\cdot) z) \geq (s_{in} - s)(u - \mu(\cdot) z)$$

and thus we have $f(s, z, u_{\max}) \geq f(s, z, u)$. As before, this implies that $s(t, t_0, s_0, 0, u_{\max}) \geq s(t, t_0, s_0, 0, u)$, up to time $t_*$. Since $\gamma$ is increasing on $[\bar{s}, s_{in}]$, we have for any admissible control $u$:

$$\gamma(s(t_0, s_0, 0, u_{\max})) \geq \gamma(s(t_0, s_0, 0, u))$$

Finally, since $\gamma$ reaches its maximum at $\bar{s}$ we get

$$K(t_0, s_0, z_0, \psi_s) = \int_{t_0}^{t_*} \gamma(s(t, t_0, s_0, 0, u_{\max})) dt + \int_{t_*}^{T} \gamma(\bar{s}) dt$$

$$\geq \int_{t_0}^{t_*} \gamma(s(t, t_0, s_0, 0, u)) dt$$

$$= K(t_0, s_0, z_0, u)$$

$\square$

6. NUMERICAL SIMULATIONS

To illustrate our results we present here numerical simulations. Figure 1 shows the dynamics of the bioreactor with the feedback (18) and figure 2 shows the cost (3) of the original problem with the feedback (18).

To illustrate the frame (9) we plot the cost (3) of the original problem with the feedback (18) along with $W_+ : s_0 \mapsto \max(0, 1) W(0, s_0, 0)$ and $W_- : s_0 \mapsto \min(0, 1) W(0, s_0, 0)$, for different fixed values of $z_0 \leq 1$ in figure 3.

We plot (figure 4)

$$\begin{cases} s_0 & \mapsto W_+(s_0, 0) - J(0, s_0, z_0, \psi_s) \\ \frac{J(0, s_0, z_0, \psi_s)}{J(0, s_0, z_0, \psi_s)} \end{cases}$$

which measures the relative error of the (suboptimal) feedback with respect to the original problem.
These simulations were done with parameters from Bernard et al. (2001) for a Haldane growth function and the parameters are: $\mu_{\text{max}} = 0.74$, $K_s = 9.28$, $K_i = 256$, $s_{\text{in}} = 100$ and $u_{\text{max}} = 1$.

For the substrate and biomass dependent case we illustrate the frame (15) in figure 5 by plotting the cost (4) of the original problem with the feedback $\hat{u}^*$ for different fixed values of $z_0$ and we compare it to $W_- : s_0 \mapsto \min(1, z_0) \tilde{W}(0, s_0, z_0)$ and $W_+ : s_0 \mapsto \max(1, z_0) \tilde{W}(0, s_0, z_0)$. Similarly, we give an example of the frame (16) in figure 6 by plotting the cost (4) of the original problem with the feedback $\hat{u}^*$ along with $W_- : s_0 \mapsto \max(1, z_0) \tilde{W}(0, s_0, z_0)$ and $W_+ : s_0 \mapsto \min(1, z_0) \tilde{W}(0, s_0, z_0)$ for different fixed values of $z_0$.

Finally, we compare the feedbacks $\hat{u}^*$ and $\tilde{u}^*$ for the cost (4) of the original problem in figure 7. In figure 8, one can see that the best strategy among $\hat{u}^*$ and $\tilde{u}^*$ depends on the initial condition $(s_0, z_0)$, as expected.

The simulations for the SBD case were done with the following parameters: $\mu_{\text{max}} = 4.5$, $K_s = 9.28$, $s_{\text{in}} = 100$ and $u_{\text{max}} = 1$.

7. CONCLUSION

In this work, we have proposed an original method to obtain a frame for the value function without the knowledge of the optimal control. Furthermore, this method enabled us to find a suboptimal feedback control law with a guaranteed value, that is within the bounds of the frame. We show that this feedback is autonomous for the substrate dependent case while it is not for the substrate and biomass dependent case.

Future prospects of this work include the generalisation of this frame method to a larger class of optimal control problems, as in Rapaport and Cartigny (2004), and regarding the maximisation of biogas, extensions of these results to 2 stage models.

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