On optimal strategies for feeding in minimal time a SBR with several species

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Abstract— **In this paper we consider the optimal control problem consisting of feeding in minimal time a Sequential Batch Reactors (SBR) where several species compete for a single substrate, with the objective being to reach a given (low) level of the substrate. Following [8, Gajardo et al. *Minimal Time Sequential Batch Reactors with Bounded and Impulse Controls for One or More Species*. SIAM J. Control and Optimization, vol. 47, Issue 6, pp. 2827-2856, 2008], we allow controls to be bounded measurable functions of time plus possible impulses. A suitable modification of the dynamics leads to a slightly different optimal control problem, without impulsive controls, for which we apply different optimality conditions derived from the Pontryagin principle and the Hamilton-Jacobi-Bellman equation. We thus characterize the singular arcs of our problem as the extremal trajectories keeping the substrate at a constant level. We also establish conditions for which a "immediate one impulse" (IOI) strategy is optimal. Some numerical experiences are then included in order to show that those conditions are also necessary to ensure the optimality of the IOI strategy.**

I. INTRODUCTION.

Sequential batch reactors (SBR) are often used in biotechnological application, notably in waste-water treatments. This device consists typically in a tank which is filled with biological micro-organisms capable to degrade some undesirable substrate. The method consists then in a sequence of cycles composed by three phases:

- Phase 1: filling the reactor with water to be treated,
- Phase 2: waiting the concentration of the undesirable substrate to decrease until a given (low) concentration,
- Phase 3: emptying the reactor from the *clean* water, leaving the sludge inside.

See [6], [8], [12], [4] for more details about the fundamental role of SBR in bioengineering.

In this study, we focus on optimal control problem consisting of feeding in minimal time a SBR where several species compete for a single substrate, the objective being to reach a given (low) level of the substrate. We consider only increasing growth functions for these species. So, our work can be seen as an extensions of some of the results obtained for one and two species in Moreno [6] and Gajardo et al. [8], respectively. For a multi-species setting, we fully characterize the existence of singular arc (which existence can lead to complex solutions that are not easily tractable from the mathematical point of view) and we study under which conditions the strategy that consists of filling as fast as possible the tank up to its maximum capacity and then waiting is optimal. This strategy is called **immediate one impulse** (IOI) in the impulsional framework developed here and it will be precisely defined in Section III.C. The last issue has been successfully solved for one single species in [6] by only assuming that the growth function is nondecreasing. However, when two species coexist in the SBR, it is shown in [8] that the fact that both growth functions are increasing is no longer enough to ensure the optimality of the IOI strategy. This result is somehow surprising. Morevoer, it is also proved therein that the IOI strategy is optimal only when one species is clearly more performant than the other one. In this paper, we go beyond this conclusion, and we discover that, in the case when more than two species coexist in the SBR, even if there is a species clearly more performant than the other ones, one cannot ensure that the IOI strategy is optimal. Indeed, the only case when we are able to prove this is when, additionally to the existence of a most performant species, the rest of the species are sufficiently close one to each other. So, this somehow captures the flavor of the two-species case.

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II. PRELIMINARIES

In this section we recall the main notions and basic results used in Gajardo, Ramírez and Rapaport [8] that constitute the basis of our work. Thus, in the next subsections we quickly describe the model and the minimal time problem involved in our analysis, we recall the equations and properties obtained from the application of Pontryagin's principle and some known results concerning the optimality of the IOI strategy.

A. Mathematical model

The dynamics of a SBR with several species can be described as follows (see [12])

$$\begin{cases} \dot{x}_i = \mu_i(s)x_i - \dfrac{F}{v}x_i,\ x_i(t_0) = y_i \\ (i = 1 \cdots n), \\ \dot{s} = -\displaystyle\sum_{j=1}^{n} \mu_j(s)x_j + \dfrac{F}{v}(s_{in} - s),\ s(t_0) = z, \\ \dot{v} = F,\ v(t_0) = w, \end{cases} \tag{II.1}$$

where x_i, s and v stand respectively for the concentration of the ith species, the concentration of the substrate and the current volume of water present in the tank. The parameter $s_{in} > 0$ is a constant which represents the substrate concentration in the input flow. The growth functions $\mu_i(\cdot)$ are non-negative smooth functions such that $\mu_i(0) = 0$, and the input flow F is a non-negative control variable.

Given a (desirable) substrate concentration $s_{out} \in]0, s_{in}[$ and a volume (of the reactor) $v_{max} > 0$, consider the domain $\mathcal{D} = (\mathbb{R}^n_+ \setminus \{0\}) \times]0, s_{in}] \times]0, v_{max}[$ and the target $\mathcal{T} = \mathbb{R}^n_+ \times]0, s_{out}] \times \{v_{max}\}$. From any initial condition $\xi = (y, z, w)$ in $\mathcal{D}$ at time t_0, the objective is to reach $\mathcal{T}$ in minimal time. This means to treat as fast as possible the maximum quantity of water, which in the case of the considered SBR is given by v_{max}. In the context of optimal control theory it leads to the following optimization problem

$$\inf_{F(\cdot)} \left\{ t - t_0 \,|\, s^{t_0,\xi,F}(t) \leq s_{out},\ v^{t_0,\xi,F}(t) = v_{max} \right\}, \quad \text{(II.2)}$$

where $s^{t_0,\xi,F}(\cdot)$, $v^{t_0,\xi,F}(\cdot)$ denote solutions of (II.1) with initial condition $\xi \in \mathcal{D}$ at time t_0 and control $F(\cdot)$.

Here $F(\cdot)$ is allowed to be a non-negative measurable function plus possible positive impulses. Indeed, instead of an ordinary control $F(\cdot)$, we consider a measure $dF(\cdot)$ that we decompose into a sum of a measure absolutely continuous with respect to the Lebesgue measure $u(t)dt$ and a singular or *impulsive* part $d\sigma$ (see [9], [10])

$$dF(t) = u(t)dt + d\sigma \ . \quad \text{(II.3)}$$

Here, $u(\cdot)$ is a measurable non-negative control that we impose to be bounded from above by u_{max}, because it corresponds to the use of a *pump* device. At time t, the non-negative *impulse* $d\sigma$ corresponds to an (instantaneous) addition of volume from $v^-(t)$ to $v^+(t)$.

From [8] we know that a time parameterization $\tau \geq t_0$ such that $dt = r(\tau)d\tau$ where

$$r(\tau) = \begin{cases} 1 & \text{when } dF \text{ is a.c. at } t(\tau), \\ 0 & \text{otherwise,} \end{cases}$$

permits to replace dynamics (II.1) by the system

$$\begin{cases} \dfrac{dx_i}{d\tau} = r\mu_i(s)x_i - \dfrac{u}{v}x_i \quad (i = 1 \cdots n) \ , \\ \dfrac{ds}{d\tau} = -r\displaystyle\sum_{j=1}^{n} \mu_j(s)x_j + \dfrac{u}{v}(s_{in} - s) \ , \\ \dfrac{dv}{d\tau} = u \ , \end{cases} \quad \text{(II.4)}$$

where the controls $u(\cdot)$ and $r(\cdot)$ are sought among measurable functions w.r.t. τ, taking values in $[0, u_{max}]$ and $\{0, 1\}$, respectively. Notice that in this formulation $u(\cdot)$ plays the both role of an ordinary control when $r = 1$ and the control of the amplitude of the jump when $r = 0$, with the same single constraint $u \in [0, u_{max}]$.

Remark 1: Since one can always take $r = 0$ and $u = 0$ on a arbitrarily large τ-interval without modifying the total time, the minimal time problem has no unique solution. Hence, we will be only interested in controls satisfying $r(\tau) \neq 0$ or $u(\tau) \neq 0$ for all time τ.

Consequently, from now on, we work with $V(\cdot)$ the value function of the reformulated problem (II.4) given by

$$V(\xi) = \inf_{(u,r)(\cdot)} \int_{t_0}^{\tau} r(\theta)d\theta \ \text{ such that} \\ s^{t_0,\xi,u,r}(\tau) \leq s_{out} \ , \ v^{t_0,\xi,u,r}(\tau) = v_{max}, \quad \text{(II.5)}$$

where $s^{t_0,\xi,u,r}(\cdot)$, $v^{t_0,\xi,u,r}(\cdot)$ denote solutions of (II.4) with initial condition $\xi \in \mathcal{D}$ at time t_0 and controls $u(\cdot)$ and $r(\cdot)$.

Remark 2: Any trajectory of the dynamics (II.4) with initial condition $\xi = (y, z, w)$ lies in the region defined by

$$\rho(\xi) = w \left(\sum_{j=1}^{n} y_j + z - s_{in} \right) \ . \quad \text{(II.6)}$$

This leads to a reduction of variables in dynamics (II.4), which will be used in Section II-C.

Now, let $G_1(\cdot)$ and $G_2(\cdot)$ be the vector fields defined by

$$G_1(\mathbf{z}(\tau)) = \left(\mu_1(s)x_1, \cdots, \mu_n(s)x_n, -\sum_{i=1}^{n} \mu_i(s)x_i, 0 \right)^\top,$$

$$G_2(\mathbf{z}(\tau)) = \left(-\tfrac{x_1}{v}, \cdots, -\tfrac{x_n}{v}, \tfrac{(s_{in}-s)}{v}, 1 \right)^\top,$$

where $\mathbf{z} = (x_1, \cdots, x_n,\ s,\ v)^\top$. Setting $u_1 = r$ and $u_2 = u$, system (II.4) is rewritten as follows

$$\dot{\mathbf{z}} = u_1 G_1(\mathbf{z}) + u_2 G_2(\mathbf{z}). \quad \text{(II.7)}$$

The formalism given by system (II.7) will be intensively exploited in the next sections.

B. Pontryagin's Minimum Principle

In this section, we establish the Pontryagin Minimum Principle (PMP) for the affine control system (II.7) on $\mathbb{R}^{n+2}$.

For our purposes it is enough to use the version of the PMP stated and proved in [11]. Recall that the principle gives a first order necessary conditions for continuous–time optimal problems.

In our particular case, the principle reads: If $\boldsymbol{u}_* = (u_{1_*}, u_{2_*})$ is an optimal control and $\mathbf{z}_*$ is the associated trajectory of (II.7) on $\mathbb{R}^{n+2}$, there exists a constant $\lambda_0 \geq 0$ and an absolutely continuous function $\boldsymbol{\lambda} : [0, T] \longrightarrow \mathbb{R}^{n+2}$, $t \mapsto \boldsymbol{\lambda}(\tau) = (\lambda(\tau), \lambda_{n+1}(\tau), \lambda_{n+2}(\tau))$ with $\lambda(\tau) = (\lambda_1(\tau), \lambda_2(\tau), \cdots, \lambda_n(\tau))$ such that for almost every $\tau \in Dom(\mathbf{z}_*)$, $(\boldsymbol{\lambda}, \lambda_0)$ never vanishing and the extremals satisfy

$$\dot{\mathbf{z}} \ = \ \tfrac{\partial \mathcal{H}}{\partial \boldsymbol{\lambda}}(\mathbf{z}, \boldsymbol{\lambda}, u_1, u_2), \quad \text{(II.8)}$$

$$\dot{\boldsymbol{\lambda}} \ = \ -\boldsymbol{\lambda}(u_1 \mathcal{J}G_1 + u_2 \mathcal{J}G_2), \quad \text{(II.9)}$$

Futhermore, the optimal control $\boldsymbol{u}_*$ minimizes the Hamiltonian

$$\mathcal{H} \ = \ u_1 \mathcal{H}_{G_1} + u_2 \mathcal{H}_{G_2} + u_1 \lambda_0 \quad \text{(II.10)}$$

over the control set, through the curve $(\boldsymbol{\lambda}(\tau), \mathbf{z}(\tau))$. Here $\mathcal{H}_{G_i}(\mathbf{z}, \boldsymbol{\lambda}) = \langle \boldsymbol{\lambda}(\tau), G_i(\mathbf{z}(\tau)) \rangle$, $i = 1, 2$, are the Hamiltonian lifts corresponding to each vector field G_i respectively. Throughout this paper we assume $\lambda_0 = 1$, which corresponds to the normal extremals.

It is well known that the Poisson bracket of the Hamiltonian functions $\mathcal{H}_{G_1}$ and $\mathcal{H}_{G_2}$, denote by $\{ \cdot, \cdot\}$, is associated with the Lie bracket by the relation

$$\{\mathcal{H}_{G_1}, \mathcal{H}_{G_2}\} = \langle \boldsymbol{\lambda}, [G_1, G_2]\rangle \tag{II.11}$$

where the Lie bracket is defined to be $[X, Y](\mathbf{z}) = \mathcal{J}Y(\mathbf{z})(X(\mathbf{z})) - \mathcal{J}X(\mathbf{z})(Y(\mathbf{z}))$ for any pair of vector fields X and Y. Here $\mathcal{J}$ stand for the Jacobian differential operator with respect to $\mathbf{z}$, and $\langle\cdot,\cdot\rangle$ is the Euclidean inner product in $\mathbb{R}^{n+2}$ (see for instance, [1]).

Now, introducing the auxiliary variables $\widetilde{\lambda}_i = \lambda_i - \lambda_{n+1}$, the adjoint system becomes the following dynamical systems

$$\tfrac{d\widetilde{\lambda}}{d\tau} = A(\tau)\widetilde{\lambda}, \quad \widetilde{\lambda}_i(T) = -1, \; i = 1, \ldots, n. \tag{II.12}$$

where $A(\tau)$ is a the $n \times n$ time dependent matrix already described in [8]. Consequently, one has

$$\widetilde{\lambda}(\tau) \neq 0 \text{ for any } \tau \in [\tau_0, T]. \tag{II.13}$$

Note that the Hamiltonian (II.10) can be equivalently written as follows

$$\mathcal{H} = u_2\phi_{u_1}(\mathbf{z}, \boldsymbol{\lambda}) + u_1\phi_{u_1}(\mathbf{z}, \boldsymbol{\lambda}) \tag{II.14}$$

where

$$\begin{cases} \phi_{u_1}(\mathbf{z}(\tau), \boldsymbol{\lambda}(\tau)) = 1 + \langle \boldsymbol{\lambda}(\tau), G_1(\mathbf{z}(\tau))\rangle, \\ \phi_{u_2}(\mathbf{z}(\tau), \boldsymbol{\lambda}(\tau)) = \langle \boldsymbol{\lambda}(\tau), G_2(\mathbf{z}(\tau))\rangle. \end{cases} \tag{II.15}$$

For the sake of simplicity, from now on, we just put $\phi_{u_i}(\tau)$ instead of $\phi_{u_i}(\mathbf{z}(\tau), \boldsymbol{\lambda}(\tau))$.

In the rest of the paper we will consider only increasing growth functions:

Assumption A1. The functions $\mu_i(\cdot)$ are non decreasing.

This assumption is quite usual in application (e.g. [6], [12]). For instance, any Monod growth function of the form $\mu(s) = \frac{\mu_{max}s}{K+s}$ (where μ_{max} and K are positive constants depending on the species) satisfies this hypothesis.

Lemma 2.1: Under Assumption A1, the following assertions hold:

(i) The matrix $A(\tau)$ has non–negative off–diagonal terms, i.e., the dynamical system (II.12) is cooperative.

(ii) The vector $m^1(\cdot)$, defined by

$$m^1(\tau) = \left(\mu_1'(s(\tau))x_1(\tau), \cdots, \mu_n'(s(\tau))x_n(\tau)\right)^\top \tag{II.16}$$

lies in $\mathbb{R}^n_+$.

Proof: The proof is direct and it was already established in [8]. □

Notice that the controls are not obviously determined by the minimum condition at times τ for which $\phi_{u_1}(\tau) = \phi_{u_2}(\tau) = 0$. Indeed, PMP is not able to distinguish minima from maxima in that periods of time. However, it is well known from the optimal control theory that optimal trajectory may be singular, that is, switching functions $\phi_{u_i}(\tau),\; i = 1, 2,$ may vanish identically along the trajectory. The characterization of such trajectories, is in general a difficult task. We will provide some general characterization in Section III.

Finally, from Proposition 6.1 in [8], we have that, along an optimal trajectory, the switching functions $\phi_{u_1}(\cdot)$ and $\phi_{u_2}(\cdot)$ defined by $(II.15)$ are related to the value function V, and consequently they are always positive for an extremal trajectory.

C. The Immediate One Impulse strategy

From an initial state $\xi = (y, z, w) \in \mathcal{D}$ at time t_0, we define the **Immediate One Impulse** strategy, which consists of making:

1. An impulse of volume $v_{max} - w$ at t_0. This can be achieved by $r(\tau) = 0$, $u(\tau) = u_{max}$, for $\tau \in [t_0, t_0 + (v_{max} - w)/u_{max}]$.

2. A null control (no feeding) until the concentration $s(\tau)$ reaches s_{out}.

For convenience, we shall denote by $\tilde{y}(\xi)$ and $\tilde{z}(\xi)$ the concentrations obtained with an impulse of volume $v_{max} - w$ from a state $\xi = (y, z, w) \in \mathcal{D}$:

$$\tilde{y}(\xi) = y\frac{w}{v_{max}}, \; \tilde{z}(\xi) = z\frac{w}{v_{max}} + s_{in}\left(1 - \frac{w}{v_{max}}\right). \tag{II.17}$$

Notice that for the particular case $\tilde{z}(\xi) \leq s_{out}$, the first step only is used.

We consider a family of functions $\varphi_c(\cdot)$ defined on $(\mathbb{R}^n_+ \setminus \{0\}) \times \mathbb{R}_+$ and parameterized by $c > 0$:

$$\varphi_c(y, z) = \inf\left\{t - t_0 \,|\, s^{t_0,y,z}(t) \leq c\right\}, \tag{II.18}$$

where $s^{t_0,y,z}(\cdot)$ is solution of the free dynamics:

$$\begin{cases} \dfrac{dx_i}{d\tau} = \mu_i(s)x_i, \quad x_i(t_0) = y_i \quad (i = 1 \cdots n), \\ \dfrac{ds}{d\tau} = -\displaystyle\sum_{i=1}^{n} \mu_i(s)x_i, \quad s(t_0) = z. \end{cases} \tag{II.19}$$

Standard analysis of minimal time problems shows that $\varphi_c(\cdot)$ are Lipschitz-continuous functions and solutions, in the viscosity sense, of the partial differential equation (see for instance [7])

$$\sum_{j=1}^{n}(\partial_{y_j}\varphi_c(y, z) - \partial_z\varphi_c(y, z))\mu_j(z)y_j + 1 = 0 \;, \tag{II.20}$$

on the domain $(\mathbb{R}^n_+ \setminus \{0\}) \times (c, +\infty)$ with boundary conditions

$$\varphi_c(., z) = 0, \quad \forall z \in (0, c]. \tag{II.21}$$

The time cost of the IOI strategy can then be simply written in terms of above functions, as follows

$$T_{IOI}(\xi) = \varphi_{s_{out}}(\tilde{y}(\xi), \tilde{z}(\xi)), \tag{II.22}$$

where $\tilde{y}(\xi)$ and $\tilde{z}(\xi)$ are given by (II.17).

Now, we assume the following regularity on the function $\varphi_c(\cdot)$,

Assumption A0. For any $c > 0$, the function $\varphi_c(\cdot)$ is C^1 on $(\mathbb{R}^n_+ \setminus \{0\}) \times (c, +\infty)$.

Remark 3: Observe that the sub-optimal IOI strategy has a finite time cost $T_{IOI}(\xi)$ for a any initial condition ξ in the domain $\mathcal{D}$. Consequently, the optimal value $V(\xi)$ is finite for any ξ in $\mathcal{D}$.

Finally, Proposition 5.3 in [8] provides a direct way to verify when the IOI strategy is optimal for any initial condition $\xi = (y, z, w) \in \mathcal{D}$. We recall here below this key tool.

Proposition 2.2: Under Assumption A0, the one impulse strategy is optimal for any $\xi \in \mathcal{D}$ if and only if

$$\Delta_{u_1} T_{IOI}(\xi) \geq 0, \ \forall\ \xi \in \mathcal{D} \ \ s.t. \ \ T_{IOI}(\xi) > 0.$$

where $\Delta_{u_1} T_{IOI}(\xi)$ is computed as follows

$$\Delta_{u_1} T_{IOI}(\xi) = \sum_{j=1}^{n} \left(\partial_{y_j}\varphi_{s_{out}}\left(\widetilde{y}(\xi), \widetilde{z}(\xi)\right) - \partial_z \varphi_{s_{out}}\left(\widetilde{y}(\xi), \widetilde{z}(\xi)\right)\right) \times \widetilde{y}_j \left(\mu_j(z) - \mu_j(\widetilde{z}(\xi))\right). \tag{II.23}$$

III. Characterization of singular arcs

In our context, a *singular arc* corresponds to an extremal curve for which there exists a nontrivial interval $[\tau_1, \tau_2] \subset [0, T]$ where both switching functions $\phi_{u_i}(\tau)$, $i = 1, 2$, are identically zero. This can be understood as an extension of the standard definition of singular arcs when only one control is considered (e.g. [5, Part III, Ch. 2]).

Since the switching functions play a crucial role in the definition of a singular arc, we proceed here below to analyze them. In particular, we focus on the computation of their derivatives.

Lemma 3.1: For dynamics (II.4), the first derivative with respect to the time τ of the switching functions $\phi_{u_i}(\tau)$, $i = 1, 2$, defined in (II.15), are given by

$$\left\{ \begin{array}{lcl} \dfrac{d\phi_{u_2}}{d\tau} & = & -u_1 \dfrac{(s_{in} - s)}{v} \langle \widetilde{\lambda}, m^1 \rangle, \\[2ex] \dfrac{d\phi_{u_1}}{d\tau} & = & u_2 \dfrac{(s_{in} - s)}{v} \langle \widetilde{\lambda}, m^1 \rangle. \end{array} \right. \tag{III.1}$$

where $\widetilde{\lambda} = (\lambda_1 - \lambda_{n+1}, ..., \lambda_n - \lambda_{n+1})$ and $m^1 = m^1(\tau)$ was defined in (II.16).

Proof: This property was shown in [8, Eq. (6.5)]. □

Denote by

$$\psi := \frac{(s_{in} - s)}{v} \langle \widetilde{\lambda}, m^1 \rangle \tag{III.2}$$

the function appearing in the first derivative of the switching functions. We now establish a formula of the n–order derivative for ψ.

Proposition 3.2: Consider a fixed time τ. For a given integer j, define $m^j = m^j(\tau)$ by

$$m^j(\tau) = \left(\mu_1^{(j)}(s(\tau))x_1(\tau), \cdots, \mu_n^{(j)}(s(\tau))x_n(\tau)\right)^\top, \tag{III.3}$$

where $\mu_i^{(j)}$ denotes the j-th derivative of μ_i with $i = 1, 2$. Then, if $\langle \widetilde{\lambda},\ m^k \rangle = 0$ for every $k = 1, \cdots, j$, we get

$$\frac{d^j \psi}{d\tau^j} = \frac{(s_{in} - s)}{v} \langle \widetilde{\lambda}, m^{j+1} \rangle \left(\frac{ds}{d\tau}\right)^j, \tag{III.4}$$

Proof: We proceed to prove the desired implication by induction on j. The case $j = 1$ follows directly from the definition of ψ given in (III.2). Now, suppose that the induction hypothesis holds true for a given j, that is, the following assertion is fulfilled: if $\langle \widetilde{\lambda},\ m^k \rangle = 0$ for every $k = 1, \cdots, j$ then (III.4) is verified. In order to establish our induction argument, we also suppose that $\langle \widetilde{\lambda},\ m^k \rangle = 0$ for every $k = 1, \cdots, j$, and we proceed to prove that equation (III.4) holds true when we replace j by $j + 1$.

The induction hypothesis implies that (III.4) holds, this yields

$$\begin{aligned} \frac{d^{j+1}\psi}{d\tau^{j+1}} &= \frac{(s_{in} - s)}{v} \left(\frac{ds}{d\tau}\right)^j \frac{d}{d\tau} \langle \widetilde{\lambda}, m^{j+1} \rangle \\ &+ \frac{d}{d\tau} \left(\frac{(s_{in} - s)}{v} \left(\frac{ds}{d\tau}\right)^j \right) \langle \widetilde{\lambda}, m^{j+1} \rangle \end{aligned} \tag{III.5}$$

On the other hand, direct computations lead to

$$\begin{aligned} \langle \widetilde{\lambda}, A(\tau)^\top m^{j+1} \rangle &= \frac{u_2}{v} \langle \widetilde{\lambda}, m^{j+1} \rangle \\ &+ u_1 \left(\sum_i \mu_i^{(j+1)} x_i \right) \langle \widetilde{\lambda}, m^1 \rangle - u_1 \langle \widetilde{\lambda}, \widetilde{m}^{j+1} \rangle \end{aligned} \tag{III.6}$$

and

$$\begin{aligned} \langle \widetilde{\lambda}, \frac{d}{d\tau} m^{j+1} \rangle &= \left(\frac{ds}{d\tau}\right) \langle \widetilde{\lambda}, m^{j+2} \rangle \\ &- \frac{u_2}{v} \langle \widetilde{\lambda}, m^{j+1} \rangle + u_1 \langle \widetilde{\lambda}, \widetilde{m}^{j+1} \rangle, \end{aligned} \tag{III.7}$$

where we have used the auxiliary notation

$$\widetilde{m}^j = \left(\mu_1^{(j)} \mu_1 x_1, \cdots, \mu_n^{(j)} \mu_n x_n\right)^\top.$$

So, equations (III.6) and (III.7) lead to

$$\begin{aligned} \frac{d}{d\tau} \langle \widetilde{\lambda}, m^{j+1} \rangle &= \langle \widetilde{\lambda}, A(\tau)^\top m^{j+1} \rangle + \langle \widetilde{\lambda}, \frac{d}{d\tau} m^{j+1} \rangle \\ &= \frac{ds}{d\tau} \langle \widetilde{\lambda}, m^{j+2} \rangle + u_1 \left(\sum_{i=1}^n \mu_i^{(j+1)} x_i \right) \langle \widetilde{\lambda}, m^1 \rangle, \end{aligned} \tag{III.8}$$

Replacing (III.8) into (III.5) we have

$$\begin{aligned} \frac{d^{j+1}\psi}{d\tau^{j+1}} &= \frac{(s_{in} - s)}{v} \left(\frac{ds}{d\tau}\right)^{j+1} \langle \widetilde{\lambda}, m^{j+2} \rangle \\ &+ u_1 \left(\frac{ds}{d\tau}\right)^j \left(\sum_{i=1}^n \mu_i^{(j+1)} x_i \right) \langle \widetilde{\lambda}, m^1 \rangle \\ &+ \frac{d}{d\tau} \left[\frac{(s_{in} - s)}{v} \left(\frac{ds}{d\tau}\right)^j \right] \langle \widetilde{\lambda}, m^{j+1} \rangle, \end{aligned} \tag{III.9}$$

Finally, since by hypothesis the two last terms in the right–hand side of (III.8) are equal to zero, it follows that

$$\frac{d^{j+1}\psi}{d\tau^{j+1}} = \frac{(s_{in}-s)}{v}\left(\frac{ds}{d\tau}\right)^{j+1} \langle\widetilde{\lambda}, m^{j+2}\rangle,$$

which proves our induction argument. □

Now we are ready to state the main result of this section.

Theorem 3.3: Consider initial condition $\xi = (y, z, w) \in \mathcal{D}$. Suppose that the matrix

$$\mathfrak{D} = \begin{pmatrix} \mu_1^{(1)}(s) & \cdots & \mu_n^{(1)}(s) \\ \mu_1^{(2)}(s) & \cdots & \mu_n^{(2)}(s) \\ \vdots & \ddots & \vdots \\ \mu_1^{(n)}(s) & \cdots & \mu_n^{(n)}(s) \end{pmatrix} \qquad \text{(III.10)}$$

is nonsingular for any $s \in (0, s_{in})$. Then, an extremal curve is a singular arc on $(\tau_1, \tau_2) \subset [0, T]$ iff $s(\cdot)$ is constant on (τ_1, τ_2).

Proof: First note that an initial condition $\xi = (y, z, w) \in \mathcal{D}$ implies that $s(\tau) \in (0, s_{in})$ for all time τ, so we will always suppose that s will remain in this interval.

Suppose that a singular arc defined in an interval of time $(\tau_1, \tau_2) \subset [0, T]$ is optimal. Since u_1 and u_2 are not simultaneously equal to zero, $\langle\widetilde{\lambda}, m^1\rangle = 0$ on (τ_1, τ_2) (via equations (III.1)); this in particular implies that the derivatives of ψ with respect to the time τ are null on (τ_1, τ_2). So, we can apply inductively Proposition 3.2 and obtain that

$$\frac{d^j\psi}{d\tau^j} = \frac{(s_{in}-s)}{v}\left(\frac{ds}{d\tau}\right)^{j} \langle\widetilde{\lambda}, m^{j+1}\rangle = 0 \qquad \text{(III.11)}$$

on (τ_1, τ_2), and for all $j = 1, 2, \cdots, n-1$.

Suppose now that $\frac{ds}{d\tau} \neq 0$. It follows from (III.11) that

$$\langle\widetilde{\lambda}, m^j\rangle = 0, \quad j = 1, \cdots, n \ \text{ on } (\tau_1, \tau_2). \qquad \text{(III.12)}$$

Hence, using the fact that $\tilde{\lambda}(\tau) \neq 0$ for all τ (see $(II.13)$), we have that $m^1, m^2, \cdots, m^n$ are linearly dependent for any $\tau \in (\tau_1, \tau_2)$. However, we have $m^j = X\eta^j$ with

$$X = \begin{pmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{pmatrix} \text{ and } \eta^j = \begin{pmatrix} \mu_1^{(j)}(s(\tau)) \\ \vdots \\ \mu_n^{(j)}(s(\tau)) \end{pmatrix}.$$

And, since X is clearly non-singular and vectors η^j's are linearly independent (because they are the rows of the matrix $\mathcal{D}$, which is non-singular), these is a contradiction with the linear dependence of m^j's. We thus conclude that $\frac{ds}{d\tau} = 0$.

Reciprocally, suppose now that $\frac{ds}{d\tau} = 0$ on (τ_1, τ_2). Equation (III.8) (with $j = 0$ for which the formula is still valid) leads to $\frac{d}{d\tau}\langle\widetilde{\lambda}, m\rangle = \varphi(\tau)\langle\widetilde{\lambda}, m\rangle$, for some given function $\varphi(\cdot)$. Hence, $\langle\widetilde{\lambda}, m\rangle = C\exp\left(\int_0^\tau \varphi(\tau)d\tau\right)$ on (τ_1, τ_2), for a real constant C.

Suppose now that $C \neq 0$. One obtains from $(III.1)$ that the switching functions ϕ_{u_1} and ϕ_{u_2} are both monotone on (τ_1, τ_2). This implies that ϕ_{u_1} and ϕ_{u_2} are both strictly positive on (τ_1, τ_2). Consequently, (II.14) implies that controls u_1 and u_2 are both equal to zero. This is a contradiction.

Therefore, the only possibility is $C = 0$. In this case, $(III.1)$ implies that the switching functions ϕ_{u_1} and ϕ_{u_2} are both constant on (τ_1, τ_2). Since u_1 and u_2 are strictly positive, it follows from Lemma 3.1 that $\phi_{u_1} = \phi_{u_2} = 0$ on (τ_1, τ_2), that is, this is a singular arc on (τ_1, τ_2). The theorem follows. □

Remark 4: The hypotheses imposing that the determinant of $\mathcal{D}$ is non null extends Assumption A2 from [8] to an arbitrary number of species. For this reason, in what follows, this condition will be also called **Assumption A2**.

A. Application: n species with a Monod growth function

In this section, we analyze the case when the growth function of each species considered in the SBR follows a Monod law. For this, as a first step, we develop here below a formula for the derivatives of a general Monod function.

Lemma 3.4: For any Monod function $\mu(s) = \frac{\mu_{max}s}{K+s}$, its derivatives with respect to s are given by

$$\mu^{(j)}(s) = \frac{(-1)^{j+1}j!K\mu_{max}}{(K+s)^{j+1}}, \text{ for all } j.$$

Proof: The proof follows directly from induction on j. □

As an application of the results obtained in this section, a characterization of singular arcs, for the case in which several species compete for the same substrate and all of them have Monod growth function, is given in the following proposition.

Proposition 3.5: Assume that each species follows a Monod law, that is

$$\mu_i(s) = \frac{\mu_{max,i}s}{K_i + s}, \quad i = 1, \cdots, n \qquad \text{(III.13)}$$

where $K_i \neq K_j$, for all $i \neq j$. Then, an extremal curve is a singular arc on $(\tau_1, \tau_2) \subset [0, T]$ if and only if $s(\cdot)$ is constant on (τ_1, τ_2).

Proof: Lemma 3.4 and some additional computations show that the determinant of the matrix $\mathcal{D}$, defined in (III.10), is given by

$$\frac{n\,[(n-1)!]^2 \prod_{l=1}^{n}\mu_{max,l} \prod_{l=1}^{n} K_l \prod_{i,j=1,\ i>j}^{n}(K_i - K_j)}{\prod_{l=1}^{n}(K_l + s)^{n+1}}.$$

Now, since $K_i \neq K_j$ for all $i \neq j$, it follows that the determinant of $\mathcal{D}$ is non null, and consequently $\mathcal{D}$ is nonsingular. Then, the desired result follows from Theorem 3.3. □

IV. Optimality of the IOI strategy

This section is devoted to the main aim of our study; to evaluate whenever the IOI strategy is optimal for our minimal time control problem. For this, the following assumption will be crucial in the sequel.

Assumption A3 For any $s_1, s_2 \in [s_{out}, s_{in}]$ and $j = 1, \cdots, n-1$, one has

$$s_2 \geq s_1 \ \Rightarrow \ \mu_n(s_2)\mu_j(s_1) \geq \mu_j(s_2)\mu_n(s_1). \qquad \text{(IV.1)}$$

Remark 5: Notice that for Monod laws of the form (III.13), implications (IV.1) are exactly fulfilled when $K_n \geq K_j$ for all $j = 1, \ldots, n-1$. Indeed, direct computations lead to

$$\mu_n(s_2)\mu_j(s_1) - \mu_j(s_2)\mu_n(s_1) = \frac{\mu_{max,n}\mu_{max,1}s_1s_2\,(s_2 - s_1)\,(K_n - K_j)}{(K_j + s_2)\,(K_j + s_1)\,(K_n + s_2)\,(K_n + s_1)}.$$

In [8] it is shown that, when only two species coexist and one is clearly more performant than the other one (which is reflected via the condition $\mu_2(s) \geq \mu_1(s)$, for all $s \in (0, s_{in}]$, on the growth functions), then the IOI strategy is optimal. Moreover, numerical experiences proved that this condition is also necessary. In other words, the fact that growth functions are increasing is not enough to ensure the optimality of the IOI strategy, which constitutes a surprising result.

Following this idea of our analysis, one would like to investigate if similar behaviors occur in the case when more than two species coexist ($n > 2$). For this, in what follows, we assume the existence of a species which is clearly more performant than the other ones. This is stated via the following assumption.

Assumption A4 Suppose that $\mu_n(s) \geq \mu_j(s), \ \forall \ j = 1, \ldots, n-1, \ s \in (0, s_{in}]$.

In this framework, next numerical example shows that Assumptions A0, A1, A3 and A4 do not ensure the optimality of the strategy IOI. In the other words, we establish the surprising result that in the case of more than two species, even the existence of a "most performant species" is not enough for this purpose.

Example: We consider the following three growth functions (See Figure 1):

$$\mu_1(s) = \frac{s}{1+s}, \ \mu_2(s) = \frac{2s}{1.5+s}, \ \mu_3(s) = \frac{4s}{2+s}.$$

They clearly fulfill Assumptions A0, A1, A2, A3 and A4. Consider also the parametric values $v_{max} = 10$, $s_{out} = 0.1$ and $s_{in} = 5$, and the initial conditions $y_1 = 1$, $y_2 = 0.001$, $z = 3$, and $w = 1$. In the Table 1 we compare, for different values of the initial condition y_3, the times achieved by the strategy IOI and by an alternative strategy, called $SA(s^*)$, introduced in articles [6], [8]. The latter consists of reaching, as fast as possible, a given level s^* in $(s_{out,s_{in}})$, then to keep s constant and equal to s^* until v reaches v_{max} and, finally, put $u = 0$ and $r = 1$ (which means to close the pump) until s reaches s_{out}. The level s^* is numerically computed here in order to minimize the cost of this type of strategies among all possible values of s^* in (s_{out}, s_{in}). Recall that in the case of two species, it was shown in [8] that this strategy was the unique other possible optimal strategy besides IOI when Assumptions A0, A1, A2, A3 and A4 were fulfilled.

So, reported results in Table 1 establish that $SA(s^*)$ has a gain close to 25% with respect to IOI for some values of y_3. We thus conclude that IOI is not optimal for this particular setting.

Table 1.

y_3	$T(IOI)$	s^*	$T(SA(s^*))$	gain
0	5.419275	–	–	–
10^{-4}	5.416174	4.226000	5.402767	0.2%
10^{-3}	5.389022	3.540000	4.978126	7.6%
10^{-2}	5.172141	3.442000	4.170769	19.4%
0.05	4.669824	3.344000	3.548414	24.0%
0.1	4.350146	3.246000	3.274169	24.7%
0.5	3.458854	3.050000	2.620281	24.2%

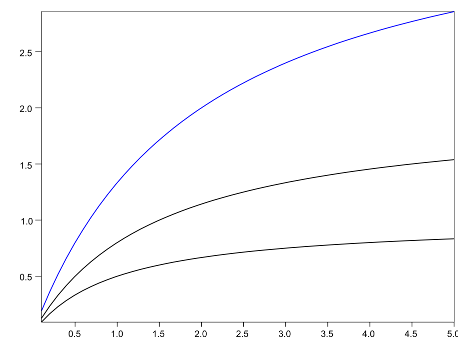

Fig. 1. Graphs of the three growth functions considered in the example.

The latter reveals another surprising and interesting result. Note that growth functions satisfy the next stronger condition than A4:

Assumption A4' $\mu_n(s) \geq \mu_{n-1}(s) \geq \cdots \geq \mu_1(s), \ \forall \ s \in (0, s_{in}]$.

This means that the performance of all the species are perfectly ordered. Thus assumption A4' can be interpreted as a stronger extension of the corresponding condition in [8]. However, the example above states that even under this stronger condition it is not possible to ensure the optimality of the IOI strategy.

Due to this negative result, we proceed to investigate other hypotheses (stronger than A4) for which one can prove that the IOI strategy is optimal. For this, at this stage of our analysis, we need to state a technical lemma for the family of functions $\varphi_c(\cdot)$. This is a direct extension of the corresponding results in [8]. Since its proof is very similar to those appearing in [8], it is omitted here.

Lemma 4.1: Under Assumptions A0, A1, A3 and A4, functions $\varphi_c(\cdot)$ posses the following properties for all $c \in (0, s_{in})$, $(y, z) \in \left(\mathbb{R}^2_+ \setminus \{0\}\right) \times (c, s_{in}]$, and $i = 1, 2, \cdots, n-1$:

i. $\partial_z \varphi_c(y,z) \geq \partial_{y_n} \varphi_c(y,z)$,

ii. $\frac{\mu_n(z)-\mu_n(\tilde{z})}{\mu_n(\tilde{z})} \leq \frac{\mu_i(z)-\mu_i(\tilde{z})}{\mu_i(\tilde{z})} \leq 0$.

Now we are in position to establish an additional condition for which IOI is optimal in this framework.

Proposition 4.2: Suppose that the Assumptions A0, A1, A3 and A4 are fulfilled. Suppose also that growth functions μ_i, for $i = 1, \ldots, n-1$, are all *close enough* one each other on $[0, s_{in}]$, that is, there exists a small enough $\epsilon > 0$ such that for all $i, j = 1, ..., n-1,\ s \in [0, s_{in}]$ one has

$$\mu_i(s) - \mu_j(s) \leq \epsilon. \tag{IV.2}$$

Then IOI strategy is optimal for any initial condition in $\mathcal{D}$.

Proof: Consider $\xi \in \mathcal{D}$ such that $T_{IOI}(\xi) > 0$. Let us denote for all $i = 1, ..., n-1$:

$$\gamma_i = \left(\frac{\mu_i(z) - \mu_i(\tilde{z})}{\mu_i(\tilde{z})} \right) / \sum_{j=1}^{n-1} \frac{\mu_j(z) - \mu_j(\tilde{z})}{\mu_j(\tilde{z})}.$$

Part ii of Lemma 4.1 ensures that $\gamma_i \geq 0$ for all i. Moreover, Hypothesis (IV.2) implies that

$$\gamma_i \in \left[\frac{1}{n-1} - \tilde{\epsilon}, \frac{1}{n-1} + \tilde{\epsilon} \right], \quad \forall i = 1, ..., n-1, \tag{IV.3}$$

for some $\tilde{\epsilon} > 0$. Note that the magnitude of $\tilde{\epsilon}$ is driven by ϵ, that is, $\tilde{\epsilon}$ can be set as small as necessary provided that ϵ is chosen small enough. Indeed, it suffices to note that $\mu_i(\tilde{z}) \geq \mu_i(z)$ and the fact that the μ_i are bounded on $[0, s_{in}]$.

Notice that the term $\Delta_{u_1} T_{IOI}(\xi)$, given in (II.23), can be written as follows

$$\Delta_{u_1} T_{IOI}(\xi) = \sum_{j=1}^{n} \Big(\partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \Big) \mu_j(\tilde{z}) \tilde{y_j} \frac{\mu_j(z) - \mu_j(\tilde{z})}{\mu_j(\tilde{z})} .$$

So, from Part ii of Lemma 4.1 and (IV.3) we obtain that $\gamma_n \geq \gamma_i \geq \frac{1}{n-1} - \tilde{\epsilon}$, for all $i = 1, ..., n-1$. Then, Part i of Lemma 4.1 implies

$$\begin{aligned}
&\frac{\Delta_{u_1} T_{IOI}(\xi)}{\sum_{j=1}^{n-1} \frac{\mu_j(z)-\mu_j(\tilde{z})}{\mu_j(\tilde{z})}} \\
&\leq \sum_{j=1}^{n-1} \left(\partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right) \mu_j(\tilde{z}) \tilde{y_j} \gamma_j \\
&+ \left(\partial_{y_n} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right) \mu_n(\tilde{z}) \tilde{y_n} \left(\frac{1}{n-1} - \tilde{\epsilon} \right) \\
&\leq \frac{1}{n-1} \sum_{j=1}^{n} \left(\partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right) \mu_j(\tilde{z}) \tilde{y_j} \\
&+ \tilde{\epsilon} \sum_{j=1}^{n} \left| \partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right| \mu_j(\tilde{z}) \tilde{y_j} \\
&= -\frac{1}{n-1} + \tilde{\epsilon} \sum_{j=1}^{n} \left| \partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right| \mu_j(\tilde{z}) \tilde{y_j} \ ,
\end{aligned}$$

where this last equality is due to (II.20). Consequently

$$\Delta_{u_1} T_{IOI}(\xi) \geq -\left(\sum_{j=1}^{n-1} \frac{\mu_j(z) - \mu_j(\tilde{z})}{\mu_j(\tilde{z})} \right) \times \left(\frac{1}{n-1} - \tilde{\epsilon} \sum_{j=1}^{n} \left| \partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right| \mu_j(\tilde{z}) \tilde{y_j} \right).$$

Therefore, since $y, \tilde{y}, z, \tilde{z}$ remain in a compact set and all the function involved are C^1, the right–hand side term in the above expression is positive provided that $\tilde{\epsilon}$ is small enough. We thus conclude thanks to Proposition 2.2. □

Note that the assumption on growth functions μ_i, for $i = 1, \ldots, n-1$, which imposes to all of them to be *close enough* to each other on $[0, s_{in}]$ (cf. (IV.2)), gets the flavor of the two-species case ($n = 2$). Indeed, it looks like we are available to ensure the optimality of IOI only when, on the one hand, one species is clearly more performant than the others and, on the other hand, the rest of the species behaves "similarly". Unfortunately, Proposition 4.2 does not provide an easy way to estimate the value ϵ, that is, it does not provide quantitative information about how close growth functions μ_i's (for $i = 1, \ldots, n-1$) should be. Indeed, in theory, it suffices to take ϵ such that the corresponding (positive) $\tilde{\epsilon}$ satisfies

$$\tilde{\epsilon} \leq \frac{1}{n-1} \ / \ \sum_{j=1}^{n} \left| \partial_{y_j} \varphi_{s_{out}}(\tilde{y}, \tilde{z}) - \partial_z \varphi_{s_{out}}(\tilde{y}, \tilde{z}) \right| \mu_j(\tilde{z}) \tilde{y_j}.$$

However, the derivatives $\partial_{y_j} \varphi_{s_{out}}$ and $\partial_z \varphi_{s_{out}}$ cannot be explicitly computed in practice. The latter is thus not useful to compute $\tilde{\epsilon}$. Hence, Proposition 4.2 should be seen just as qualitative information on μ_i's concerning the optimality of IOI strategy.

V. Conclusions

In this paper, we have studied the optimal control problem consisting of feeding in minimal time a SBR where several species compete for a single substrate, the objective being to reach a given (low) level of the substrate. We consider only increasing growth functions for these species.

For this multi-species setting, we have fully characterized the existence of singular arcs. Also, we have studied under which conditions the IOI strategy is optimal. We have thus obtained that, one the one hand, this strategy is optimal when one species is clearly more performant than the others and the rest of the species are sufficiently close one to each other (which can be seen as these species behaves "similarly") and, on the other hand, the existence of a more performant species is not enough to ensure the optimality of the IOI strategy. The latter has been shown via numerical experiences.

So, it seems that the optimality of the IOI strategy is strongly related to the two species case developed in [8]. Indeed, if we can identify a cluster of microorganisms with similar behavior and which is less performant than the other species, this cluster can be roughly speaking treated as one single species. Then the result obtained for two species in [8] can be extended properly to this setting. When this cannot be done because the species of this cluster are not "close enough" (or equivalently, they do not behave similarly), then results obtained therein, as well as the optimality of IOI strategy, are no longer true. We believe that this qualitative information is very valuable when one considers water treatment with SBR's.

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