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ANALYSIS OF AN OPTIMAL CONTROL PROBLEM CONNECTED TO BIOPROCESSES INVOLVING A SATURATED SINGULAR ARC

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ABSTRACT. We study a minimal time control problem under the presence of a saturation point on the singular locus. The system describes a fed-batch reactor with one species and one substrate. Our aim is to find an optimal feedback control steering the system to a given target in minimal time. The growth function is of Haldane type implying the existence of a singular arc which is non-necessary admissible everywhere (i.e. the singular control can take values outside the admissible control set). Thanks to Pontrygin's Principle, we provide an optimal synthesis of the problem that exhibits a frame point at the intersection of the singular arc and a switching curve. Numerical simulations allow to compute this curve and the frame point.

1. Introduction. Minimal time control problems for affine systems with one input such as:

$$\dot{x} = f(x) + ug(x), \quad x \in \mathbb{R}^n, \quad |u| \leq 1, \quad (1)$$

have been investigated a lot in the literature, see e.g. [9, 10, 20, 21, 28, 29, 30] and [8] for $n = 2$ and references herein. One often encounters singular trajectories which appear when the switching function of the system is vanishing on a time interval. In order to find an issue to a minimal time control problem governed by (1), one usually requires that the singular control u_s is admissible, which means that

$$|u_s| \leq 1. \quad (2)$$

This allows the trajectory to stay on the singular arc. However, one cannot in general show that this assumption holds. In fact, the expression of the singular control in terms of the state and adjoint state does not always guarantee that (2) is satisfied. One can argue that it is enough to consider a larger admissible upper bound for the controls, but this seems rather artificial, and not necessarily feasible from a practical point of view. The objective of this work is to study a minimal time control problem in the plane where the singular control satisfies (2) only on a sub-domain of the state space (the part of the singular arc where (2) does not hold

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is usually called *barrier* [8, 9, 10, 20, 21]). This may happen in many engineering problems in particular when the singular control can take arbitrary large values in the state space.

The system that we consider is a fed-batch bioreactor with one species and one substrate [19]. Our aim is to find an optimal feedback control that steers the system in minimal time to a given target where the substrate concentration is less than a prescribed value, see [19]. Finding an optimal feeding strategy can significantly increase the performance of the system and has several advantages from a practical point of view (see e.g. [1, 2, 6, 7, 12, 13, 14, 16, 19]). The design of adequate feedback control laws is used for instance in wastewater treatment industries [13].

Whenever the growth function is of Monod type [18, 26], then one can prove that the optimal feeding strategy is bang-bang [19]. This means that the reactor is filled until its maximum volume with the maximum input flow rate. Then, micro-organisms consume the substrate until reaching a reference value. In the case where the growth function is of Haldane type (in case of substrate inhibition [18, 26]), this strategy is no longer optimal. In fact, one can prove that the optimal strategy is *singular* provided that the singular arc is always admissible (see [19]). It consists in reaching in minimal time a substrate concentration \bar{s} corresponding to the maximum of the growth rate function, and which coincides with the singular set. Then, the substrate concentration is kept constant at this value until reaching the maximal volume (a more detailed description of singular strategies can be found in [1, 2, 12, 19]).

In the present work, we are interested in studying the optimal synthesis for Haldane-type growth function whenever the singular arc is no longer admissible from a certain volume value. This can happen when the singular control becomes larger than the maximal input flow rate which is allowed in the system. It follows that there exists a volume value above which singular extremal trajectories are no longer admissible. Such a point is usually called *saturation point* [5, 15, 23, 24]. Whereas in [1, 19], the maximal volume can be reached by a singular trajectory, this is no longer possible as the singular control saturates before reaching this value.

In this setting, the optimal synthesis of the problem is more intricate to obtain as one cannot apply the clock form (see [4]). Thanks to the Pontryagin's Principle, we provide an optimal synthesis of the problem. In particular, we show that singular optimal trajectories leave the singular arc at a *frame point* defined as the intersection between the singular arc and a switching curve (see [8] for a description of frame points). As a consequence, a singular extremal trajectory ceases to be optimal before reaching the saturation point. This phenomena is studied in [8, 20, 23, 24] where local results are given. In [23], a local regular synthesis is given in low dimension for the minimal time problem with the saturation phenomena. It appears in several systems such as a model of tumor-cancer therapy [15, 24], in the problem of NMR [5], and in chemical engineering when optimizing a batch reactor (i.e. without input substrate) w.r.t. the temperature [7, 6].

The paper is organized as follows. The second section states the optimal control problem. We also recall the optimality result of [19] and we apply Pontryagin's Principle. The third section is devoted to the optimal synthesis of the problem whenever the singular arc is not admissible. In Proposition 4, we show that optimal controls are of type *BSBB* or *BBSB* with at most three switching points (here *B* denotes a bang arc and *S* a singular arc). Proposition 2 studies the case where the singular arc is never admissible in the state space. This allows to obtain an optimal

feedback control of the problem (see Theorems 3.2 and 3.3) in line with [15, 23, 24]. In section 4, we provide numerical simulations of optimal trajectories and computations of the switching curve and the frame point. Several questions on the optimal synthesis are discussed in the last section (implicit equation of the switching curve, regularity of the value function, and uniqueness of optimal trajectories).

2. General results. In this section, we state the optimal control problem and we recall the optimal synthesis as in [19] that will allow us to introduce the optimal control problem when the singular arc is partially admissible. We also apply the Pontryagin Maximum Principle (PMP) [22] that will be used in the next section.

2.1. Statement of the problem. We consider a system describing a fed-batch bioreactor with one species and one substrate [14, 26]:

$$\begin{cases} \dot{x} = x \left(\mu(s) - \frac{u}{v} \right), \\ \dot{s} = -\mu(s)x + \frac{u}{v}(s_{in} - s), \\ \dot{v} = u. \end{cases} \quad (3)$$

Here x represents the concentration of micro-organisms (biomass), s the concentration of substrate, and v is the volume of the tank. The input substrate concentration is denoted by $s_{in} > 0$, and u is the input flow rate in the system. For convenience, we have taken a yield coefficient equal to one (by rescaling the equation). The function $s \mapsto \mu(s)$ is the growth function of Monod or Haldane type (see [18, 26]). In the following, we consider that u takes values within the set:

$$\mathcal{U} := \{u : [0, +\infty) \rightarrow [0, u_{max}] ; u \text{ meas.}\}.$$

Here u_{max} denotes the maximum input flow rate in the system. By time scaling, we can take $u_{max} = 1$. The target we consider is defined by:

$$\mathcal{T} := \mathbb{R}_+^* \times [0, s_{ref}] \times \{v_m\},$$

where s_{ref} is a given substrate concentration (typically s_{ref} is such that $s_{ref} \ll s_{in}$ in wastewater treatment). For $u \in \mathcal{U}$, let $t_{\xi_0}(u)$ the time to steer (3) from an initial condition $\xi_0 := (x_0, s_0, v_0) \in \mathbb{R}_+^* \times [0, s_{in}] \times [0, v_m]$. The optimal control problem becomes:

$$\inf_{u \in \mathcal{U}} t_{\xi_0}(u), \text{ s.t. } \xi(t(u)) \in \mathcal{T}, \quad (4)$$

where $\xi(\cdot)$ denotes the unique solution of (3) for the control u that starts at ξ_0 . One essential feature in the system (3) is that the quantity

$$M := v(x + s - s_{in}), \quad (5)$$

is conserved along any trajectory of (3), hence M is constant and equal to $v_0(x_0 + s_0 - s_{in})$. From (5), we obtain:

$$x = \frac{M}{v} + s_{in} - s, \quad (6)$$

and system (3) can be put into a two-dimensional system:

$$\begin{cases} \dot{s} = -\mu(s) \left(\frac{M}{v} + s_{in} - s \right) + \frac{s_{in} - s}{v} u, \\ \dot{v} = u. \end{cases} \quad (7)$$

One can easily show that the set $[0, s_{in}] \times \mathbb{R}_+^*$ is invariant by (7). Notice that if we define x by (6), the micro-organisms concentration may not be positive. This can happen when $M \leq 0$ which means that initial conditions of micro-organisms and

substrate are low. Therefore, we consider initial conditions for (7) in the domain \mathcal{D} defined by:

$$\mathcal{D} := \left\{ (s, v) \in [0, s_{in}] \times (0, v_m] ; \frac{M}{v} + s_{in} - s > 0 \right\}.$$

We denote by $\partial\mathcal{D}$ the boundary of \mathcal{D} . In the rest of the paper, we also write $u(\cdot)$ a control in open loop and $u[\cdot]$ a feedback control depending on the state (s, v) . Also, we define two vector fields $f, g : \mathcal{D} \rightarrow \mathbb{R}^2$ associated to (7) by:

$$f(s, v) := \begin{bmatrix} -\mu(s)\left(\frac{M}{v} + s_{in} - s\right) \\ 0 \end{bmatrix}, \quad g(s, v) := \begin{bmatrix} \frac{s_{in}-s}{v} \\ 1 \end{bmatrix}.$$

2.2. Optimal synthesis in presence of an admissible singular arc. In this part, we review a result of [19] on optimal trajectories for problem (4) in the case where the singular arc is always admissible. First, we consider the case where the growth function μ is of Monod type i.e. $\mu(s) = \frac{\bar{\mu}s}{k+s}$ with $\bar{\mu} > 0$ and $k > 0$ [18].

Theorem 2.1. *Assume that μ is of Monod type. Then, the optimal feedback control u_M steering any initial condition in \mathcal{D} to the target \mathcal{T} is:*

$$u_M[s, v] := \begin{cases} 1 & \text{if } v < v_m, \\ 0 & \text{if } v = v_m. \end{cases}$$

In other words, the optimal strategy is *fill and wait*, and it consists in filling the tank with maximum input flow rate until $v = v_m$, and then we let $u = 0$ until s reaches the value s_{ref} (if necessary). In the rest of the paper, we only consider the case where the growth function μ is of *Haldane type* i.e.

$$\mu(s) = \frac{\bar{\mu}s}{gs^2 + s + k},$$

with $\bar{\mu} > 0$, $g > 0$, and $k > 0$. In this case, μ has exactly one maximum over \mathbb{R}_+ , that we denote \bar{s} , and we suppose that $\bar{s} > s_{ref}$ (which means that the reference concentration to achieve is sufficiently small). The optimal synthesis in this case is rather different than for Monod growth function (see an illustration Fig. 4).

Theorem 2.2. *Assume that μ is of Haldane type and that the following assumption holds:*

$$\mu(\bar{s}) \left[\frac{M}{s_{in} - \bar{s}} + v_m \right] \leq 1. \quad (8)$$

Then, the optimal feedback control u_H to reach the target is given by

$$u_H[s, v] := \begin{cases} 0 & \text{if } v = v_m \quad \text{or} \quad s > \bar{s}, \\ 1 & \text{if } s < \bar{s} \quad \text{and} \quad v < v_m, \\ u_s[v] & \text{if } s = \bar{s} \quad \text{and} \quad v < v_m, \end{cases}$$

where

$$u_s[v] := \mu(\bar{s}) \left[\frac{M}{s_{in} - \bar{s}} + v \right]. \quad (9)$$

This can be proved by using either the PMP or the clock form [4, 17]. Here we have emphasized that (8) is necessary in order to state the optimality result (see e.g. [1, 12]). The control u_s is *singular* (see section 2.3). It allows to maintain the substrate concentration equal to \bar{s} . It can be written $u_s[v] = \frac{\mu(\bar{s})x}{v(s_{in}-\bar{s})}$ so that

$u_s \geq 0$. Therefore, (8) is essential to ensure that $u_s[v]$ satisfies the upper bound $u_s[v] \leq 1$ for all $v \leq v_m$.

The objective of this paper is to provide an optimal synthesis of the problem whenever (8) is not satisfied. From (9), one can see that the singular control can take arbitrary large values. Note that in practice, one should start the fed-batch with a high biomass concentration (i.e. high M) in order to speed up the process, so that condition (8) can no longer be satisfied.

2.3. Pontryagin maximum principle. In this part we apply the PMP on (4). The existence of an optimal control is straightforward from standard arguments. First, notice that any trajectory of the system takes values within the compact set $[0, s_{in}] \times [0, v_m]$. Moreover, a trajectory corresponding to the feedback u_M steers any initial condition to the target. As the system is affine w.r.t. the control which takes values within a compact set, the result follows. Let $H := H(s, v, \lambda_s, \lambda_v, \lambda_0, u)$ the Hamiltonian of the system defined by:

$$H := -\lambda_s \mu(s) \left[\frac{M}{v} - (s - s_{in}) \right] + u \left[\frac{\lambda_s (s_{in} - s)}{v} + \lambda_v \right] + \lambda_0.$$

If u is an optimal control and $z := (s, v)$ the corresponding solution of (7), there exists $t_f > 0$, $\lambda_0 \leq 0$, and an absolutely continuous map $\lambda = (\lambda_s, \lambda_v) : [0, t_f] \rightarrow \mathbb{R}^2$ such that $(\lambda_0, \lambda) \neq 0$, $\dot{\lambda}_s = -\frac{\partial H}{\partial s}$, $\dot{\lambda}_v = -\frac{\partial H}{\partial v}$, that is:

$$\begin{cases} \dot{\lambda}_s = \lambda_s \left(\mu'(s)x - \mu(s) + \frac{u}{v} \right), \\ \dot{\lambda}_v = \lambda_s \left(\frac{-\mu(s)M + u(s_{in} - s)}{v^2} \right), \end{cases} \quad (10)$$

and we have the maximality condition:

$$u(t) \in \arg \max_{\omega \in [0, 1]} H(s(t), v(t), \lambda_s(t), \lambda_v(t), \lambda_0, \omega), \quad (11)$$

for almost every $t \in [0, t_f]$. We call *extremal trajectory* a sextuplet $(s(\cdot), v(\cdot), \lambda_s(\cdot), \lambda_v(\cdot), \lambda_0, u(\cdot))$ satisfying (7)-(10)-(11), and *extremal control* the control u associated to this extremal trajectory. As t_f is free, the Hamiltonian is zero along an extremal trajectory. Following [1], one can prove that λ_s is always non-zero (it is therefore of constant sign from the adjoint equation), and that $\lambda_0 < 0$ (hence we take $\lambda_0 = -1$ in the following). Next, let us define the *switching function* ϕ associated to the control u by:

$$\phi := \frac{\lambda_s (s_{in} - s)}{v} + \lambda_v. \quad (12)$$

We obtain from (11) that any extremal control satisfies the following control law: for a.e. $t \in [0, t_f]$, we have

$$\begin{cases} \phi(t) < 0 \implies u(t) = 0 & \text{(No feeding),} \\ \phi(t) > 0 \implies u(t) = 1 & \text{(Maximal feeding),} \\ \phi(t) = 0 \implies u(t) \in [0, 1]. \end{cases}$$

We say that t_0 is a *switching point* if the control u is non-constant in any neighborhood of t_0 which implies that $\phi(t_0) = 0$. Whenever the control u switches either from 0 to 1 or from 1 to 0 at time t_0 , we say that the control is *bang-bang* around t_0 . We will write B_0 a bang arc $u = 0$ and B_1 a bang arc $u = 1$. Whenever ϕ is zero on a non-trivial interval $I \subset [0, t_f]$, we say that u is a *singular control*, and that the trajectory contains a *singular arc*. We will write S a singular arc defined on a time

interval. The sign of $\dot{\phi}$ is fundamental in order to obtain the optimal synthesis. By taking the derivative of ϕ , we get:

$$\dot{\phi} = \frac{\lambda_s x(s_{in} - s) \mu'(s)}{v}. \quad (13)$$

Moreover, we can show that $\lambda_s < 0$ (see e.g. [1, 12]). This implies that any extremal trajectory satisfies the property:

$$s(t) > \bar{s} \implies \dot{\phi}(t) > 0; \quad s(t) < \bar{s} \implies \dot{\phi}(t) < 0. \quad (14)$$

Now, if an extremal trajectory contains a singular arc on some time interval $I := [t_1, t_2]$, then we have $\phi = \dot{\phi} = 0$ on I , hence we have $\mu'(s) = 0$ and $s = \bar{s}$ on I , hence the singular locus is the line segment $S := \{\bar{s}\} \times [0, v_m]$. By solving $\dot{s} = 0$, we obtain the expression of the singular control given by (9), see e.g. [2]. Now, along a singular arc, one has easily:

$$\ddot{\phi} = \frac{\lambda_s x(s_{in} - s) \mu''(\bar{s})}{v} \dot{s}. \quad (15)$$

As $\lambda_s < 0$ and $\mu''(\bar{s}) < 0$, one obtains from (15) that $\langle \lambda(t), [g, [f, g]](z(t)) \rangle > 0$ where $[f, g]$ denotes the Lie bracket of f and g (recall that $[f, g](z) := \frac{\partial g}{\partial z}(z)f(z) - \frac{\partial f}{\partial z}(z)g(z)$). This shows that *Legendre-Clebsch necessary condition*

$$\frac{\partial}{\partial u} \frac{d^2}{dt^2} \frac{\partial H}{\partial u}(z(t), \lambda(t), -1, u(t)) > 0,$$

is satisfied along a singular trajectory (see e.g. [15] or [11]). Again using that $\mu''(\bar{s}) < 0$, one obtains immediately that $\det(g(z(t)), [g, [f, g]](z(t))) > 0$ and that $\det(f(z(t)), g(z(t))) < 0$ which shows that the singular arc is *hyperbolic* or time minimizing [4, 3].

Remark 1. In other words, the singular arc is a turnpike [8] (this can be also verified using the clock form argument).

Finally, one obtains the time of a singular trajectory by integrating the ODE $\dot{v} = u_s$ (see e.g. [1]). Let $t_s(v_0, v_1)$ be the time of a singular extremal steering (\bar{s}, v_0) to (\bar{s}, v_1) , $v_0 < v_1$. One obtains:

$$t_s(v_0, v_1) = \frac{1}{\mu(\bar{s})} \ln \left(\frac{M + v_1[s_{in} - \bar{s}]}{M + v_0[s_{in} - \bar{s}]} \right). \quad (16)$$

3. Optimal synthesis in the general case. In this part, we provide a description of optimal trajectories for problem (4) when (8) is not satisfied. We first introduce a partition of \mathcal{D} that will allow us to describe where optimal trajectories have a switching point.

3.1. Partition of the domain \mathcal{D} . In view of (8) that can be equivalently written $v_m \leq \frac{1}{\mu(\bar{s})} - \frac{M}{s_{in} - \bar{s}}$, we introduce a mapping $\eta : (0, s_{in}) \rightarrow \mathbb{R}$ by

$$\eta(s) := \frac{1}{\mu(s)} - \frac{M}{s_{in} - s}.$$

By definition of η , we have:

$$u_s[v] = 1 \iff v = \eta(s).$$

Now, if we define a point v^* by $v^* := \eta(\bar{s})$, the singular arc is admissible provided that $v^* \geq v_m$. In the following, we make the following assumption on v^* :

(H1) We suppose that $v^* < v_m$.

Following [5, 8, 15], the point (\bar{s}, v^*) is usually called *saturation point*. It follows that the singular arc is admissible only if the volume is less than v^* i.e. the admissible part of the singular arc is $\{\bar{s}\} \times [0, v^*]$. Indeed, for $v > v^*$ equality (9) no longer defines a control in $[0, 1]$. Next, we will consider the two following cases:

- Case 1: $v^* \leq 0$,
- Case 2: $0 < v^* < v_m$.

Remark 2. Case 1 means that the singular arc is never admissible over $(0, v_m]$. As the function η can take negative values, v^* can be negative.

We now introduce curves that are solutions of (7) with $u = 1$ that will provide a partition of initial states.

Definition 3.1. We define $\hat{\mathcal{C}}$, resp. $\check{\mathcal{C}}$ as the restriction to the set \mathcal{D} of the orbit of system (7) with $u = 1$ that passes through the point (\bar{s}, v_m) , resp. (\bar{s}, v^*) .

Hence, $\hat{\mathcal{C}}$ is the graph of a C^1 -mapping $v \mapsto \hat{\gamma}(v)$ that is the unique solution of the equation:

$$\frac{ds}{dv} = -\mu(s) \left[\frac{M}{v} + s_{in} - s \right] + \frac{s_{in} - s}{v}, \quad (17)$$

over $(0, v_m]$ (recall that the point $(\bar{s}, v_m) \in \partial\mathcal{D}$) with initial condition $\hat{\gamma}(v_m) = \bar{s}$. Similarly, $\check{\mathcal{C}}$ is the graph of a C^1 -mapping $v \mapsto \check{\gamma}(v)$ that is the unique solution of (17) over $(0, v_m]$ such that $\check{\gamma}(v^*) = \bar{s}$.

The curves $\hat{\mathcal{C}}$ and $\check{\mathcal{C}}$ will play a major role in the optimal synthesis contrary to the case where the singular arc is admissible (see Fig. 3 and Table 1 for parameter values). In fact, they will indicate sub-domains where optimal trajectories have a switching point, and the existence of a frame point [8] depending on the value of M (see Hypothesis (H2) in section 3.3).

As \mathcal{D} is not backward invariant by (7), we call \hat{v} , resp. \check{v} the first volume value such that $\hat{\gamma}(\hat{v}) \notin (0, s_{in})$, resp. $\check{\gamma}(\check{v}) \notin (0, s_{in})$. We now investigate monotonicity properties of $\hat{\gamma}$ and $\check{\gamma}$ (see Fig. 1 and 3).

Proposition 1. (i) *The curve $\hat{\gamma}$ is either decreasing on $[\hat{v}, v_m]$, either there exists a unique $v_1 \in (\hat{v}, v_m)$ such that $\hat{\gamma}(v_1) \in (0, s_{in})$ and $\frac{d\hat{\gamma}}{dv}(v_1) = 0$. Moreover, in the latter case, $\hat{\gamma}$ is increasing on $[\hat{v}, v_1]$ and is decreasing on $[v_1, v_m]$.*

(ii) *The mapping $\check{\gamma}$ is increasing on $(\check{v}, v^*]$ and decreasing on $[v^*, v_m]$, and $\frac{d\check{\gamma}}{dv}(v^*) = 0$.*

Proof. Let us first prove (i). For $v \in (\hat{v}, v_m]$, we can rewrite (17) as follows:

$$\frac{ds}{dv} = \frac{\mu(s)(s_{in} - s)}{v} [\eta(s) - v].$$

When $v = v_m$, we have $\eta(\hat{\gamma}(v_m)) = \eta(\bar{s}) = v^* < v_m$, therefore, we have $\frac{d\hat{\gamma}}{dv} < 0$ in a neighborhood of v_m . Now, if $\hat{\gamma}$ is non-monotone on (\hat{v}, v_m) , then necessarily $v \mapsto \frac{d\hat{\gamma}}{dv}$ is vanishing on $(\hat{v}, v_m]$. Assume that there exist $0 < v_2 < v_1 < v_m$ such that $\hat{\gamma}(v_1) \in (0, s_{in})$, $\hat{\gamma}(v_2) \in (0, s_{in})$ and $\frac{d\hat{\gamma}}{dv}(v_1) = \frac{d\hat{\gamma}}{dv}(v_2) = 0$. Without any loss of generality, we can assume that v_i , $i = 1, 2$ are the two first zeros of $v \mapsto \frac{d\hat{\gamma}}{dv}$. Hence, we have $\eta(s(v)) > v$ for $v \in (v_2, v_1)$ so that $\frac{d\hat{\gamma}}{dv}(v) > 0$. This gives using $\eta(\hat{\gamma}(v_2)) = v_2$:

$$\eta(\hat{\gamma}(v)) - \eta(\hat{\gamma}(v_2)) > v - v_2, \quad v \in (v_2, v_1),$$

and by dividing by $v - v_2$ (with $v > v_2$), we obtain that $\frac{d}{dv} \eta(\hat{\gamma}(v))|_{v=v_2} \geq 1$. On the other hand, we find $\eta'(\hat{\gamma}(v_2)) \frac{d\hat{\gamma}}{dv}(v_2) = 0$, which gives a contradiction. Therefore,

there exists at most one value v_1 for which $\frac{d\hat{\gamma}}{dv}(v_1) = 0$, and $\hat{\gamma}(v_1) \in (0, s_{in})$. Also, by derivating (17) and using the fact that $\frac{d\hat{\gamma}}{dv}(v_1) = 0$ we get:

$$\frac{d^2\hat{\gamma}}{dv^2}(v_1) = -\frac{\mu(\hat{\gamma}(v_1))(s_{in} - \hat{\gamma}(v_1))}{v_1},$$

which is non-zero. In fact, we have seen that $\hat{\gamma}(v_1) > 0$. Moreover we have $\hat{\gamma}(v_1) \neq s_{in}$ from (17) (if $M \neq 0$, then $\frac{d\hat{\gamma}}{dv}(v_1) \neq 0$ whenever $\hat{\gamma}(v_1) = s_{in}$; if $M = 0$, then, $\hat{\gamma}(v) < s_{in}$ for all v by Cauchy-Lipschitz Theorem). We deduce that at point v_1 , the monotonicity of $\hat{\gamma}$ is changing. The conclusion of (i) follows.

Let us prove (ii). By definition of v^* , we have $\frac{d\hat{\gamma}}{dv}(v^*) = 0$. By a similar argument as for (i), one can prove that v^* is the unique zero of $v \mapsto \frac{d\hat{\gamma}}{dv}(v)$ on $(\hat{v}, v_m]$. Thus $v \mapsto \zeta(v) := \eta(\hat{\gamma}(v)) - v$ has exactly one zero on $(\hat{v}, v_m]$. Moreover, we find $\frac{d\zeta}{dv}(v^*) = -1$, therefore ζ is decreasing in a neighborhood of v^* . It follows that $\hat{\gamma}$ is increasing on $[\hat{v}, v^*]$ and decreasing on $[v^*, v_m]$, and the result follows. \square

Remark 3. (i) Proposition 1 (ii) implies that the curve \hat{C} leaves the domain \mathcal{D} through the line-segment $\{0\} \times [0, v_m]$, see Fig 3.

(ii) Proposition 1 (i) implies that the curve \hat{C} leaves the domain \mathcal{D} either through the line-segment $\{0\} \times [0, v_m]$, the line segment $[0, s_{in}] \times \{0\}$ or through the line-segment $\{s_{in}\} \times [0, v_m]$, see Fig. 1.

(iii) We can show that there exist values of M for which the cases mentioned in the previous item occur. In fact, by changing v into $w := -\ln v$, (17) can be gathered into a planar dynamical system. The stable manifold Theorem (see e.g. [26]) shows that $\lim_{v \rightarrow 0} \hat{\gamma}(v)$ is either finite or $\pm\infty$. When this limit is $\pm\infty$, $\hat{\gamma}$ leaves \mathcal{D} through $\{0\} \times [0, v_m]$ or $\{s_{in}\} \times [0, v_m]$. We have not detailed this point for brevity.

(iv) For instance, if $M = 0$, Cauchy-Lipschitz Theorem implies $\lim_{v \rightarrow 0} \hat{\gamma}(v) = -\infty$.

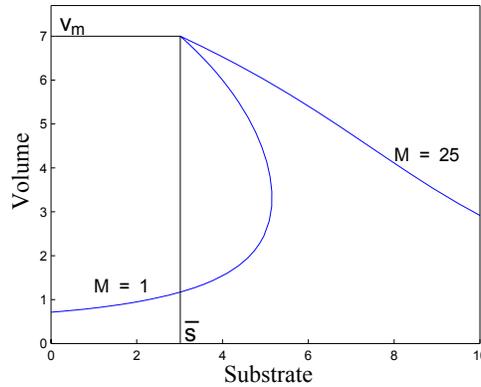


FIGURE 1. The curve \hat{C} leaves the domain \mathcal{D} through $\{0\} \times [0, v_m]$ when $M = 1$. In this case, $\hat{\gamma}$ is increasing over $[\hat{v}, v_1]$ and decreasing over $[v_1, v_m]$. The curve \hat{C} leaves the domain \mathcal{D} through $\{s_{in}\} \times [0, v_m]$ when $M = 25$. In this case, $\hat{\gamma}$ is decreasing over $[\hat{v}, v_m]$ (see Proposition 1).

When M is such that $\lim_{v \rightarrow 0} \hat{\gamma}(v) = -\infty$, the trajectory leaves the domain \mathcal{D} through the line-segment $\{0\} \times [0, v_m]$. Hence, there exists a volume value v_* such

that $\hat{\gamma}(v_*) = \bar{s}$, see Fig. 1. From the definition of v^* , the volume v_* necessarily satisfies $0 < v_* < v^*$. In fact, for any volume value v such that $v^* < v \leq v_m$, one has $\frac{ds}{dt}|_{u=1}(\bar{s}) < 0$, thus $\hat{\mathcal{C}}$ necessarily intersects the singular arc below v^* .

3.2. Optimal synthesis in the case $v^* \leq 0$. When the singular arc is never admissible, we have the following optimality result (see also Fig. 3).

Proposition 2. *Suppose that $v^* \leq 0$ (case 1). Then, given initial states $(s_0, v_0) \in \mathcal{D}$, optimal controls satisfy the following:*

- (1) *If $s_0 \leq \bar{s}$, then, there exists $t_0 > 0$ such that $u = 1$ on $[0, t_0]$, $u = 0$ on $[t_0, t_f]$ where t_0 is such that $v(t_0) = v_m$ and $s(t_f) = s_{ref}$.*
- (2) *If $s_0 > \bar{s}$, then, there exists $t_0 > 0$ such that $u = 0$ on $[0, t_0]$, $u = 1$ on $[t_0, t_1]$, $u = 0$ on $[t_1, t_f]$ where $t_0 \geq 0$, $\bar{s} < s(t_0) < s_0$, $v(t_1) = v_m$, and $s(t_f) = s_{ref}$.*

Proof. Consider an optimal trajectory $(s(\cdot), v(\cdot), u(\cdot))$ starting at an initial point $(s_0, v_0) \in \mathcal{D}$. In the present case, the control u can only take the value 0 or 1 from the PMP (the singular arc is not admissible in \mathcal{D}).

First, assume $s_0 \leq \bar{s}$. Given the assumption $v^* \leq 0$, we can show that $s(t) \leq \bar{s}$ for all t . We thus have $u = 1$ in a neighborhood of $t = 0$. Otherwise, we would have $u = 0$ together with $\phi(0) \leq 0$, and from (14) we would have for all t , $\phi(t) < 0$ which is not possible (as the trajectory would not reach the target). It follows that we have $u = 1$ in a neighborhood of $t = 0$. The same argument shows that the trajectory cannot switch to $u = 0$ before reaching v_m . This proves the first item.

Assume now that $s_0 > \bar{s}$. If $\phi(0) < 0$, then we have $u = 0$, and the trajectory necessarily switches to $u = 1$ before reaching \bar{s} (otherwise we would have a contradiction by the previous case). Now, we have $u = 1$ on some time interval $[t_0, t_1]$. Again, the previous case shows that the trajectory cannot switch to $u = 0$ at some time t' such that $s(t') \leq \bar{s}$ with $v(t') < v_m$. As $\phi(t_0) \geq 0$ and $\dot{\phi}(t) > 0$ whenever $s(t) > \bar{s}$ (recall (14)), we obtain that the trajectory cannot switch to $u = 0$ at some time t'' such that $s(t'') > \bar{s}$. Therefore, we have $u = 1$ until v_m , and the conclusion follows. \square

Remark 4. If s_0 is such that $s_0 > \hat{\gamma}(v_0)$, then we have $u = 0$ on some time interval $[0, t_0]$ with $t_0 > 0$. Otherwise we would have $\phi(0) > 0$ implying $\phi(t) > 0$ for all t (recall (14)). As the trajectory necessarily has a switching point when reaching $v = v_m$, we have a contradiction.

The previous proposition allows to define a *switching curve* $\mathcal{C} \subset \mathcal{D}$ where the control is switching from 0 to 1. Such a curve is the locus of *conjugate points* where the extremal trajectory ceases to be optimal [3]. Hence, for each $v \in (0, v_m]$ there exists at most one point $s_c(v)$ such that \mathcal{C} is parameterized by the mapping $v \mapsto s_c(v)$.

Proposition 3. *The switching curve \mathcal{C} originates from the point (\bar{s}, v_m) .*

Proof. Let $(s_0, v_0) \in \mathcal{D}$ and consider an extremal trajectory with $u = 1$ from (s_0, v_0) until reaching v_m . Recall that $\hat{\gamma}$ is a solution of (7) backward in time with $u = 1$ starting from (\bar{s}, v_m) . From Proposition 2, we must have $s_0 \leq \hat{\gamma}(v_0)$.

Suppose now that the switching curve crosses $v = v_m$ at some point (s', v_m) with $s' > \bar{s}$. Consider an extremal trajectory with $u = 1$ until $v = v_m$ originating from \mathcal{C} . If the initial condition of this extremal is sufficiently close to (s', v_m) , then it reaches v_m at a substrate value which is greater than \bar{s} . This is a contradiction with (14). Hence, $s' \leq \bar{s}$.

Now, suppose that $s' < \bar{s}$. Take an initial condition (s_0, v_0) above \mathcal{C} in the plane (s, v) and such that $s_0 < \bar{s}$, $v_0 > v_a$. From Proposition 2, one has $u = 0$ until reaching \mathcal{C} . But, any extremal trajectory starting with $u = 0$ at an initial condition $s_0 < \bar{s}$ and $v_0 < v_m$ is not optimal. Hence, we obtain a contradiction with (14) which proves the result. \square

The curve \mathcal{C} is depicted on Fig. 3. Propositions 2 and 3 allow to obtain an optimal feedback control of the problem in this case.

Theorem 3.2. *Suppose that $v^* \leq 0$ (case 1). Then the optimal feedback steering any initial state in \mathcal{D} to the target is given by:*

$$u_1[s, v] := \begin{cases} 0 & \text{if } s \geq s_c(v) \quad \text{or} \quad v = v_m, \\ 1 & \text{if } s < s_c(v) \quad \text{and} \quad v < v_m. \end{cases}$$

Proof. The result follows from Proposition 2 and the presence of the switching curve \mathcal{C} . \square

The optimal synthesis in this case is depicted on Fig. 4.

Remark 5. When the singular arc is never admissible, optimal controls are of type $B_0B_1B_0$ or B_1B_0 depending on the initial points. Optimal trajectories contain at most two switching points.

3.3. Optimal synthesis in the case $v^* \in (0, v_m)$. Throughout the paper, we only consider case 2, that is v^* is such that $0 < v^* < v_m$. We make the following assumption on M :

(H2) The constant M is such that there exists a unique v_* satisfying $0 < v_* < v^*$ and $\hat{\gamma}(v_*) = \bar{s}$.

One can see that for initial conditions (s_0, v_0) such that $v_0 > v^*$, optimal controls are given by proposition 2. Indeed, the admissible part of the singular arc is only defined for $v_0 \leq v^*$. Therefore, we consider initial states such that $v_0 < v^*$. The next Proposition is illustrated on Fig. 3.

Proposition 4. *Suppose $v^* \in (0, v_m)$ (case 2) and that (H2) is satisfied. Then, given initial states $(s_0, v_0) \in \mathcal{D}$ such that $v_0 < v^*$, optimal controls satisfy the following:*

- (1) *If $s_0 \leq \tilde{\gamma}(v_0)$, then, there exists $t_0 > 0$ such that we have $u = 1$ on $[0, t_0]$, $u = 0$ on $[t_0, t_f]$ where t_0 is such that $v(t_0) = v_m$.*
- (2) *If $\tilde{\gamma}(v_0) < s_0 < \hat{\gamma}(v_0)$ and $s_0 \leq \bar{s}$, then, there exists $t_0 > 0$ such that we have $u = 1$ on $[0, t_0]$, $u = u_s$ on $[t_0, t_1]$, $u = 1$ on $[t_1, t_2]$, $u = 0$ on $[t_2, t_f]$, where $s(t_0) = \bar{s}$, $t_1 - t_0 \geq 0$, $v(t_1) < v^*$, and $v(t_2) = v_m$.*
- (3) *If $\hat{\gamma}(v_0) \leq s_0 < \bar{s}$, then, there exists $0 < t_0 < t_1 < t_2$ such that we have $u = 1$ on $[0, t_0]$, $u = u_s$ on $[t_0, t_1]$, $u = 1$ on $[t_1, t_2]$, $u = 0$ on $[t_2, t_f]$ where $s(t_0) = \bar{s}$, $v(t_1) \in (v_*, v^*)$, $v(t_2) = v_m$.*
- (4) *If $s_0 \geq \bar{s}$ and $v_0 \leq v_*$, then, there exists $0 < t_0 < t_1 < t_2$ such that we have $u = 0$ on $[0, t_0]$, $u = u_s$ on $[t_0, t_1]$, $u = 1$ on $[t_1, t_2]$, $u = 0$ on $[t_2, t_f]$ where $s(t_0) = \bar{s}$, $v(t_1) \in (v_*, v^*)$, and $v(t_2) = v_m$.*
- (5) *If $s_0 \geq \bar{s}$, and $v_0 > v_*$, then, the optimal control is one of the following types:*
 - *either $u = 0$ on $[0, t_0]$, $u = u_s$ on $[t_0, t_1]$, $u = 1$ on $[t_1, t_2]$, $u = 0$ on $[t_2, t_f]$ where $s(t_0) = \bar{s}$ and $0 < t_0 < t_1$, $v(t_2) = v_m$,*
 - *either $u = 0$ on $[0, t_0]$, $u = 1$ on $[t_0, t_1]$, $u = 0$ on $[t_1, t_f]$ where $t_0 \geq 0$, $\bar{s} < s(t_0) < \hat{\gamma}(v_0)$, $v(t_1) = v_m$.*

Proof. The proof of the first item is the same as the first one of the previous Proposition.

Now, when $\hat{\gamma}(v_0) < s_0 < \hat{\gamma}(v_0)$ and $s_0 \leq \bar{s}$, the trajectory cannot switch from $u = 1$ to $u = 0$ before reaching $s = \bar{s}$. Therefore, we have two cases when the trajectory reaches $s = \bar{s}$: the trajectory either crosses the singular arc, or the control becomes singular. In the latter, the trajectory switches to $u = 1$ before reaching v^* and we have $u = 1$ until $v = v_m$ (otherwise we would have $u = 0$ at the point (\bar{s}, v^*) and the trajectory would not reach the target from (14)). Notice that $t_1 = t_0$ is possible. This means that the time interval where the trajectory is singular can be zero.

If $\hat{\gamma}(v_0) < s_0 < \bar{s}$, the proof is the same as for the second item except that the trajectory cannot leave the singular arc with $u = 1$ before v_* (otherwise the trajectory reaches $v = v_m$ with $u = 1$ and $\phi > 0$, and the trajectory cannot switch to $u = 0$ at $v = v_m$ from (14)).

The proof of the fourth item is the same as the third one except that the trajectory starts with $u = 0$ until reaching the singular arc. Similarly as in the previous item, the trajectory cannot switch to $u = 1$ before reaching $s = \bar{s}$.

The last region is given by initial conditions such that $s_0 \geq \bar{s}$, and $v_0 > v_*$. The same arguments as before can be used except that Pontryagin's Principle is not sufficient to exclude two type of trajectories. First observe that we have $u = 0$ on some time interval $[0, t_0]$ as before (with $s(t_0) < \hat{\gamma}(v_0)$, otherwise the trajectory would not reach the target from (14)). When the trajectory crosses the curve $\hat{\gamma}$, we have two sub-cases. Either the trajectory switches to $u = 1$ before reaching $s = \bar{s}$ (as in Proposition 2), either the trajectory switches to the singular arc for $s = \bar{s}$. After the first switching times, the behavior of the trajectory is exactly as for the second item, and we can conclude from the other cases. \square

Remark 6. Proposition 4 shows that optimal controls are of type B_1B_0 , $B_0B_1B_0$ or $B_0SB_1B_0$ with at most three switching points depending on the initial point.

We now investigate the loss of optimality of the singular arc. More precisely, we show that when the singular arc saturates at v^* , it is no longer optimal until v^* (see e.g. [8, 9, 20, 23, 24] and [5, 7, 15] for a study of the saturation phenomena). To be self contained, we provide a proof of this result in our setting.

Proposition 5. *Suppose $v^* \in (0, v_m)$ (case 2) and that (H2) is satisfied. Then, any optimal trajectory containing a singular arc leaves this singular arc between v_* and v^* (bounds not included).*

Proof. If the trajectory leaves the singular arc for a volume value less than v_* , then, we have $u = 1$ until reaching $v = v_m$. From Proposition 4, we have $\phi > 0$ at $v = v_m$ in contradiction with the fact that the trajectory switches to $u = 0$. Hence, it leaves the singular arc for a volume value $v > v_*$. Notice that if a singular trajectory reaches $v = v^*$ at a time t' , then we have $\phi(t') = \dot{\phi}(t') = 0$. For $t > t'$, we have $s(t) < \bar{s}$ for any control u (this follows from the definition of v^*). Hence, we have $\dot{\phi}(t) < 0$, and we deduce that $\phi(t) < 0$ for $t > t'$. Hence we have $u = 0$ using (11). As the trajectory necessarily has a switching point in order to reach the target, we obtain a contradiction. \square

We denote by v_a the maximal volume value above which a singular arc is not optimal. From the synthesis of singularities in [8], the point (\bar{s}, v_a) is a *frame point* of type $(CS)_2$ which means that it is at the intersection between a singular arc and

a switching curve denoted by \mathcal{C} . The index 2 means that the switching curve \mathcal{C} is originating from the singular arc. Hence, for each $v \in (v_a, v_m]$ there exists at most one point $s_c(v)$ such that \mathcal{C} is parameterized by the mapping $v \mapsto s_c(v)$.

Proposition 6. *The switching curve \mathcal{C} connects (\bar{s}, v_a) and (\bar{s}, v_m) .*

Proof. Let $(s_0, v_0) \in \mathcal{D}$ and consider an extremal trajectory with $u = 1$ from (s_0, v_0) until reaching v_m . Recall that $\hat{\gamma}$ is a solution of (7) backward in time with $u = 1$ starting from (\bar{s}, v_m) . From Proposition 2, we must have $s_0 \leq \hat{\gamma}(v_0)$.

Suppose now that the switching curve crosses $v = v_m$ at some point (s', v_m) with $s' > \bar{s}$. Consider an extremal trajectory with $u = 1$ until $v = v_m$ originating from \mathcal{C} . If the initial condition of this extremal is sufficiently close to (s_c, v_m) , then it reaches v_m at a substrate value which is greater than \bar{s} . This is a contradiction with (14). Hence, $s' \leq \bar{s}$.

Now, suppose that $s' < \bar{s}$. Take an initial condition (s_0, v_0) above \mathcal{C} in the plane (s, v) and such that $s_0 < \bar{s}$, $v_0 > v_a$. From Proposition 2, one has $u = 0$ until reaching \mathcal{C} . But, any extremal trajectory starting with $u = 0$ at an initial condition $s_0 < \bar{s}$ and $v_0 < v_m$ is not optimal. Hence, we obtain a contradiction with (14) which proves the result. \square

The switching curve \mathcal{C} is depicted on Fig. 3. Propositions 4, 5 and 6 imply the following.

Theorem 3.3. *Suppose $v^* \in (0, v_m)$ (case 2) and that (H2) is satisfied. Then, the optimal feedback steering any initial state in \mathcal{D} to the target is given by:*

$$u_2[s, v] := \begin{cases} 0 & \text{if} & v = v_m \\ 0 & \text{if} & s > s_c(v) \quad \text{and} \quad v_m > v \geq v_a, \\ 1 & \text{if} & s \leq s_c(v) \quad \text{and} \quad v_m > v \geq v_a, \\ 0 & \text{if} & s > \bar{s} \quad \text{and} \quad v < v_a, \\ 1 & \text{if} & s < \bar{s} \quad \text{and} \quad v < v_a, \\ u_s[v] & \text{if} & s = \bar{s} \quad \text{and} \quad v < v_a. \end{cases}$$

Proof. From Proposition 6, we know that an optimal trajectory does not contain a singular arc for $v \geq v_a$. It follows from Proposition 4 that the optimal feedback control is 0 or 1 depending on the position of the initial point w.r.t. the switching curve. Moreover, when $v = v_m$, the only possibility for u is zero. For $v < v_a$, the result follows from Proposition 4. \square

The optimal synthesis in this case is depicted on Fig. 4. We see that for initial conditions such that $v < v_a$, the optimal feedback is as in Theorem 2.2 whereas for $v > v_a$, the feedback control is either 0 or 1 depending where the point (s, v) is located w.r.t. the switching curve $v \mapsto s_c(v)$.

4. Numerical simulations.

4.1. Determination of the frame point. We start by computing the optimal volume value $v_a \in (v_*, v^*)$ above which the singular arc is no longer optimal. As we know the structure of optimal controls from Proposition 4, we proceed as follows. For $v_0 \in [v_*, v^*]$, consider the strategy $u = u_s$ from v_* to v_0 , $u = 1$ until v_m and

then $u = 0$ until s_{ref} . The time $t_a(v_0)$ of this strategy is (recall (16), see also [1]):

$$t_a(v_0) = \frac{\ln\left(\frac{M+v_0(s_{in}-\bar{s})}{M+v_*(s_{in}-\bar{s})}\right)}{\mu(\bar{s})} + v_m - v_0 + \int_{s_{ref}}^{s^\dagger(v_0)} \frac{d\sigma}{\mu(\sigma)\left(\frac{M}{v_m} + s_{in} - \sigma\right)}, \quad (18)$$

where $s^\dagger(v_0)$ is the substrate concentration when this trajectory reaches $v = v_m$: it is defined as the value for $v = v_m$ of the solution of (17) that starts at $s = \bar{s}$ with $v = v_0$. Hence, $s^\dagger(v_0)$ can be computed after solving the Cauchy problem:

$$\frac{ds}{dv} = -\mu(s) \left[\frac{M}{v} + s_{in} - s \right] + \frac{s_{in} - s}{v}, \quad s(v_0) = \bar{s}. \quad (19)$$

We now show that $v_0 \mapsto t_a(v_0)$ admits a minimum $v_a \in [v_*, v^*]$ that we will characterize hereafter. First, (19) can be equivalently written as $\frac{ds}{dv} = g(v, s)$ where g is the right hand-side of (19). By the classical dependence of the solution of an ODE on parameters, we denote by $s(v, \bar{s}, v_0)$ the unique solution of (19). It is standard that $v_0 \in \mathbb{R}_+^* \mapsto s(v, \bar{s}, v_0)$ is of class C^1 for all $v > 0$. It follows by composition that $v_0 \mapsto t_a(v_0)$ is of class C^1 on $[v_*, v^*]$. Consequently, it admits a minimum on this interval. By differentiating $s(v, \bar{s}, v_0)$ w.r.t. v_0 , we get:

$$\frac{\partial s}{\partial v_0}(v, \bar{s}, v_0) = -g(v_0, \bar{s}) e^{\int_{v_0}^v \frac{\partial g}{\partial s}(s(w, v_0, \bar{s}), w) dw},$$

using a classical result on the dependance w.r.t. initial conditions of a solution of an ordinary differential equation. Hence $\frac{ds^\dagger}{dv_0}(v_0) = \frac{\partial s}{\partial v_0}(v_m, \bar{s}, v_0)$.

Now, we know from the PMP that $v_0 = v^*$ and $v_0 = v_*$ are not admissible (see also Proposition 4), hence v_a necessarily satisfies $\frac{dt_a}{dv_0}(v_a) = 0$. So, if we put $\theta(v_0) := \int_{v_0}^{v_m} \frac{\partial g}{\partial s}(w, s(w, \bar{s}, v_0)) dw$, we obtain by taking the derivative of (18) w.r.t. v_0 :

$$\frac{dt_a}{dv_0}(v_0) = \frac{v^* - v_0}{\frac{M}{s_{in}-\bar{s}} + v_0} \left[1 - \frac{\mu(\bar{s})\left(\frac{M}{v_0} + s_{in} - \bar{s}\right)}{\mu(s^\dagger)\left(\frac{M}{v_m} + s_{in} - \bar{s}\right)} e^{\theta(v_0)} \right]$$

By solving $\frac{dt_a}{dv_0}(v_0) = 0$ using the previous equation, we obtain numerically the volume $v_a \in (v_*, v^*)$ above which extremal trajectories stop to be optimal. We find that $t_a(v)$ has a unique minimum for $v_a \simeq 1.67$ (see Fig. 2 and Table 1 for the values of the parameters)

4.2. Determination of the switching curve. To determine the optimal switching time for the trajectories $B_0B_1B_0$ starting with $s_0 > \bar{s}$, we proceed as follows. For each $v_0 \in (v_*, v_m)$, we search numerically $s_c(v_0) \in [\bar{s}, \hat{\gamma}(v_0)]$ which minimizes the time $t_b(\xi)$ to reach the target starting from $(\hat{\gamma}(v_0), v_0)$ with the strategy: $u = 0$ until ξ , $u = 1$ until v_m , $u = 0$ until s_{ref} . The application $\xi \mapsto t_b(\xi)$ can be written:

$$t_b(\xi) = \int_{\xi}^{\hat{\gamma}(v_0)} \frac{d\sigma}{\mu(\sigma)\left(\frac{M}{v_0} + s_{in} - \sigma\right)} + v_m - v_0 + \int_{s_{ref}}^{\xi^\dagger} \frac{d\sigma}{\mu(\sigma)\left(\frac{M}{v_m} + s_{in} - \sigma\right)},$$

where $\xi \in [\bar{s}, \hat{\gamma}(v_0)]$ and ξ^\dagger is the solution of (17) that starts at point (ξ, v_0) evaluated at $v = v_m$. Numerical simulations indicate that for each value of v_0 , the point $s_c(v_0)$ where t_b is minimal is unique. This allows us to define a curve \mathcal{C} whose graph is the mapping $v_0 \mapsto s_c(v_0)$, represented in green on Fig. 3. Moreover, we find that for $v_0 < v_a$, we have $s_c(v_0) = \bar{s}$, while $s_c(v_0) > \bar{s}$ for $v_0 \in (v_a, v_m)$. To conclude, based on the optimal synthesis (Proposition 4) and the computations of the mapping

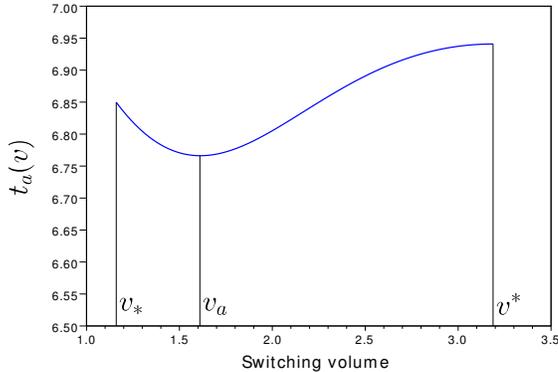


FIGURE 2. Time $t_a(v)$ to reach the target from (\bar{s}, v_*) with the strategy: singular arc until the switching volume v , $u = 1$ until v_m , $u = 0$ until s_{ref} . We find that $t_a(v)$ has a unique minimum for $v = v_a$ (see Section 4)

$v_0 \mapsto s_c(v_0)$ and v_a , optimal trajectories for various initial conditions (s_0, v_0) are represented on Fig. 3.

TABLE 1. Parameter values (arbitrary units) of simulations for the optimal synthesis when the singular arc is partially admissible (see Fig. 3 and 2)

v_m	s_{in}	s_{ref}	M	$\bar{\mu}$	k	g
7	10	0.1	25 (case 1)	0.5	1	0.11
			1 (case 2)			

Figure 4 depicts the optimal synthesis in the three cases $v^* \geq v_m$ (as in Theorem 2.2), $v^* \leq 0$ (as in Theorem 3.2), and $v^* > 0$ (as in Theorem 3.3).

5. Discussion on the optimal synthesis.

5.1. Implicit equation of the switching curve. We present a convenient way to obtain the switching curve \mathcal{C} as a solution of an implicit equation using the ODE satisfied by the switching function ϕ . From (13) and the conservation of the Hamiltonian along an extremal trajectory, we get:

$$\dot{\phi} = \rho(s, v)(u\phi - 1), \quad (20)$$

where $\rho(s, v) := \frac{(s_{in}-s)\mu'(s)}{\mu(s)v}$ and (s, v) is a solution of (7) with a control $u \in \mathcal{U}$. Define the mapping $(w, s_0, v_0) \in (0, v_m] \times \mathcal{D} \mapsto s(w, s_0, v_0)$ as the unique solution of (17) such that $s(v_0, s_0, v_0) = s_0$. From Theorem 3.3, an optimal trajectory of type $B_0B_1B_0$ starting at some point (s_0, v_0) with $v_0 < v_m$ satisfies $u = 0$ until reaching \mathcal{C} , and then $u = 1$ until reaching the volume v_m . These conditions together with (20) will imply conditions on the point (s_0, v_0) . More precisely, we have the following result.

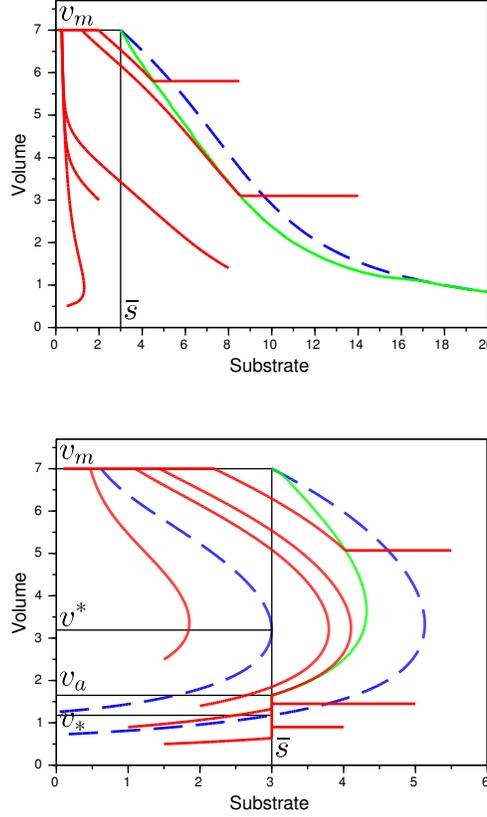


FIGURE 3. Optimal trajectories (in solid red lines) for various initial conditions. *Above*: case 1 ($v^* \leq 0$), see Proposition 2 ; *Below*: case 2 ($0 < v^* < v_m$), see Proposition 4. In blue dashed lines, trajectories $\hat{\mathcal{C}}$ and $\tilde{\mathcal{C}}$ which pass through (\bar{s}, v^*) and (\bar{s}, v_m) . In green, the switching curve \mathcal{C} which passes through (\bar{s}, v_m) in both cases and through the frame point (\bar{s}, v_a) in case 2.

Proposition 7. *Consider an extremal trajectory of type B_1 defined on a time interval $[0, t_0]$ where 0 and t_0 are two consecutive switching points i.e. $\phi(0) = \phi(t_0) = 0$. Then, the point (s_0, v_0) belongs to the switching curve if and only if $F(s_0, v_0) = 0$, where $F : \mathcal{D} \rightarrow \mathbb{R}$ is defined by:*

$$F(s_0, v_0) := \int_{v_0}^{v_m} \rho(s(w, s_0, v_0), v_0) dw.$$

Proof. By considering ϕ as a function of v (recall that $\frac{dv}{dt} = 1$ on $[0, t_0]$), one obtains:

$$\frac{d\phi}{dv} = \rho(s(v, s_0, v_0), v)(\phi - 1).$$

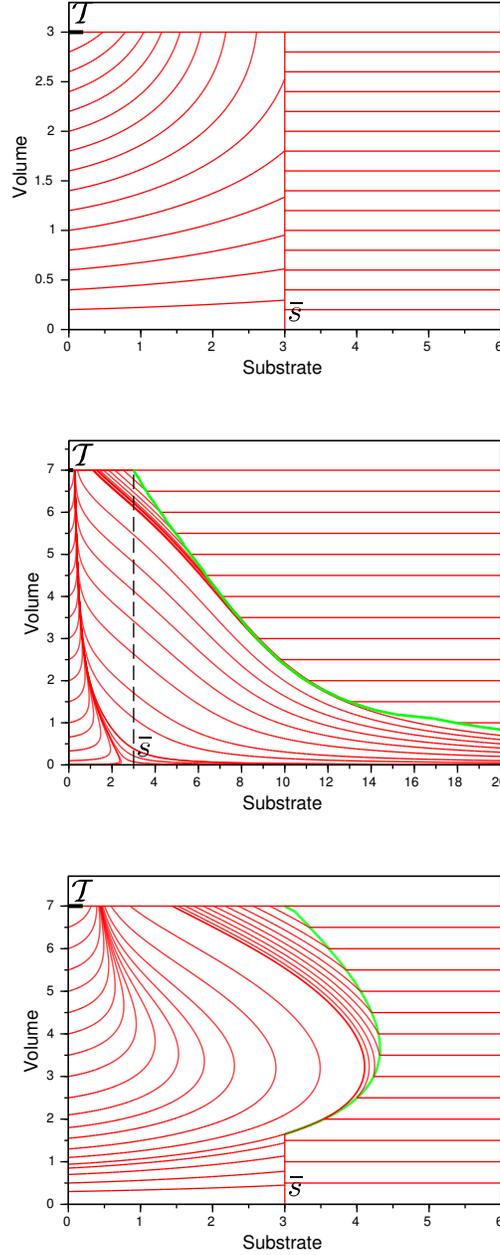


FIGURE 4. Optimal trajectories. *Above:* case $v^* \geq v_m$ (optimal synthesis provided by Theorem 2.2); *Middle:* case $v_* \leq 0$ (optimal synthesis provided by Theorem 3.2); *Below:* $v^* \in (0, v_m)$ (optimal synthesis provided by Theorem 3.3).

By integrating this equation over $[v_0, v_m]$, the initial point (s_0, v_0) must satisfy

$$\int_{v_0}^{v_m} \rho(s(v, s_0, v_0), v_0) dv = 0,$$

which gives the desired result. \square

As a consequence, determining the switching curve amounts to solve the implicit equation $F(s_0, v_0) = 0$ in \mathcal{D} for a given volume value v_0 .

Remark 7. (i) One can verify that $\frac{\partial F}{\partial s_0}(\bar{s}, v_m) \neq 0$ implying that the curve \mathcal{C} is locally the graph of a C^1 -mapping $v_0 \mapsto s_c(v_0)$ in a neighborhood of (\bar{s}, v_m) in \mathcal{D} . (ii) Solving numerically the equation $F(s_0, v_0) = 0$ for $v_0 \in [v_a, v_m]$ provides the same switching curve as the one computed in section 4.2.

5.2. Continuity of the value function. In this part, we explicit the value function $T(s, v)$ over \mathcal{D} which is associated to the minimal time problem, and we show that it is continuous. We suppose that hypotheses (H1)-(H2) are satisfied and we recall that \mathcal{C} is the switching curve connecting (\bar{s}, v_a) and (\bar{s}, v_m) . We define a curve ζ as the union of the singular arc (until v_a) and \mathcal{C} :

$$\zeta := ((\{\bar{s}\} \times [0, v_a]) \cap \mathcal{D}) \cup \mathcal{C}.$$

For $(s, v) \in \mathcal{D}$ and $0 < s' < s$, we introduce the following functions:

$$\begin{aligned} \tau_1(v) &:= \frac{1}{\mu(\bar{s})} \ln \left(\frac{M + v_a(s_{in} - \bar{s})}{M + v(s_{in} - \bar{s})} \right) + T(\bar{s}, v_a), \\ \tau_2(s', s, v) &:= \int_{s'}^s \frac{d\sigma}{\mu(\sigma) \left(\frac{M}{v} + s_{in} - \sigma \right)}. \end{aligned}$$

The function τ_1 is the time of an optimal trajectory starting on the singular arc at a volume value $v < v_a$ (recall (16)). It is clearly continuous over \mathcal{D} . The function τ_2 is the time of an extremal trajectory with $u = 0$ connecting the points (s, v) and (s', v) with $s' < s$. Clearly, it is continuous w.r.t. $(s', s, v) \in [0, s_{in}] \times \mathcal{D}$.

Let us now consider an extremal trajectory with $u = 1$ starting from a point $(s, v) \in \mathcal{D}$:

- If the trajectory reaches the concentration \bar{s} before the volume v_m , we denote by $v_1(s, v)$ the volume value of this extremal when the concentration equals \bar{s} .
- If the trajectory reaches the volume v_m before the concentration \bar{s} , we denote by $s_m(s, v)$ the substrate concentration of this extremal when the volume equals v_m .

By the regularity of an ODE w.r.t. initial conditions, these two functions are continuous on \mathcal{D} . Finally, consider the restriction to the set \mathcal{D} of the mapping $s \mapsto v_2(s)$ which is the unique solution of (7) backward in time starting at (\bar{s}, v_a) . The value function $T(s, v)$ can be now defined as follows (recall Theorem 3.3):

$$T(s, v) = \begin{cases} v_1(s, v) - v + \tau_1(v_1(s, v)) & \text{if } v \leq v_2(s) \text{ and } s < \bar{s} \\ \tau_2(\bar{s}, s, v) + \tau_1(v) & \text{if } v \leq v_a \text{ and } s \geq \bar{s} \\ v_m - v + \tau_2(s_{ref}, s_m(s, v), v_m) & \text{if } v > v_2(s) \text{ and } s < s_c(v) \\ \tau_2(s_c(v), s, v) + v_m - v + \tau_2(s_{ref}, s_m(s_c(v), v), v_m) & \text{if } v > v_a \text{ and } s \geq s_c(v) \end{cases} \quad (21)$$

Proposition 8. *The function T is continuous in \mathcal{D} .*

Proof. One can easily verify that T is continuous at any point (s, v) outside the curve ζ . Hence, we only verify its continuity on this curve.

First case. Suppose $v_0 < v_a$, and let us show that T is continuous at (\bar{s}, v_0) . If $s < \bar{s}$ and $v \leq v_2(s)$, one has $v_1(s, v) \rightarrow v_0$ whenever s goes to \bar{s} and v goes to v_0 . So, we have $T(s, v) = v_1(s, v) - v + \tau_1(v_1(s, v)) \rightarrow \tau_1(v_0)$. On the other hand, if $s > \bar{s}$ and $v \leq v_a$, one has $\tau_2(\bar{s}, s, v) \rightarrow 0$ when s goes to \bar{s} . Hence, we also obtain that $T(s, v) \rightarrow \tau_1(v_0)$ when s goes to \bar{s} and v goes to v_0 , $s > \bar{s}$.

Second case. Suppose $v_0 > v_a$, and let us show that T is continuous at the point $(s_c(v_0), v_0)$. Notice that when $s > s_c(v)$ and $v \geq v_a$, one has that $\tau_2(s_c(v), s, v) \rightarrow 0$ when $s \rightarrow s_c(v)$ which together with the expression of T (for $v > v_2(s)$ and $s < s_c(v)$) proves the result.

Third case. Suppose that $v_0 = v_a$. Then, if $v > v_2(s)$ and $s < s_c(v)$, we have $T(s, v) \rightarrow T(\bar{s}, v_a)$ when $s \rightarrow \bar{s}$ and $v \rightarrow v_a$ using that $T(\bar{s}, v_a) = v_m - v_a + \tau_2(s_{ref}, s_m(s_c(v_a), v_a), v_m) = \tau_1(v_a)$. When $v < v_2(s)$ and $s < \bar{s}$, one also has $T(s, v) \rightarrow \tau_1(v_a)$. Finally, we obtain the same limit for T when (s, v) goes to (\bar{s}, v_a) with $s > \bar{s}$. This ends the proof. \square

Remark 8. (i) The expression (21) allows to show that the value function T is of class C^1 whenever the singular arc is always admissible i.e. $v^* \geq v_m$. This result is in line with the same result in the impulsive setting [1, 14]. The expressions of $\frac{\partial T}{\partial s}$ and $\frac{\partial T}{\partial v}$ are delicate to handle in particular along an arc $u = 1$, so we have not detailed this point for brevity.

(ii) When the singular arc is no longer admissible i.e. $v^* < v_m$, we can show that T is not differentiable along the switching curve \mathcal{C} (but it is right and left differentiable on \mathcal{C}).

5.3. Regularity of the optimal synthesis. Given the feedback controls u_i , $i = 1, 2$ (see Theorem 3.2 and 3.3), we would like to know if trajectories corresponding to this feedback are unique [21]. In the case where the singular arc is always admissible [19], then one can use the clock form [4, 8] to conclude directly on the uniqueness of an optimal trajectory starting at some point $(s_0, v_0) \in \mathcal{D}$. In fact, this argument shows directly that any other trajectory has a greater cost as the optimal one (with equality only if both associated controls are equal a.e.). Hence, optimal trajectories corresponding to the feedback u_M and u_H are unique (Theorems 2.1 and 2.2).

This method no longer applies in the case where the singular arc is non admissible. Nevertheless, Pontryagin's Principle allows to exclude any extremal trajectory that has a switching point outside the singular arc $\{\bar{s}\} \times [0, v_a]$ and the switching curve, before reaching the maximal volume (see Propositions 2 and 4). These trajectories exactly correspond to the solution of (7) with the feedback control u_i .

6. Conclusion. We have studied an optimal control problem for a fed-batch bio-process that exhibits a singular arc with a saturating point. Thanks to Pontryagin's Principle and the exclusion of extremal trajectories that are not optimal, we have obtained an optimal synthesis of the problem. We have pointed out the existence of a frame point on the singular arc above which any singular trajectory is not globally optimal. Moreover, we have provided an explicit way for computing numerically the switching curves and the frame point. The present situation can arise for example when the initial biomass concentration in the reactor is high. In this case, one should take advantage of the feedback control law for the practical implementation.

A more detailed insight into the determination of the switching curves (for instance using the theory of conjugate points [3]) could be the basis of future works.

Also, it could be interesting to study an optimal synthesis of the problem with multiple saturating turnpikes [1] (this can happen in practice when there exist more than two non-limiting substrates in the reactor). This question appears to be quite challenging.

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