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Optimal synthesis for the minimum time control problems of fed-batch bioprocesses for growth functions with two maxima

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Abstract

We address the problem of finding an optimal feedback control for feeding a fed-batch bioreactor with one species and one substrate from a given initial condition to a given target value in a minimal amount of time. Recently, the optimal synthesis (optimal feeding strategy) has been obtained in systems in which the microorganisms involved are represented by increasing growth functions or growth functions with one maxima, with either Monod or Haldane functions, respectively (widely used in bioprocesses modeling). In the present work, we allow impulsive controls corresponding to instantaneous dilutions, and we assume that the growth function of the microorganism present in the process has exactly two local maxima. This problem has been considered from a numerical point of view in [15] without impulsive controls. In this article, we introduce two singular arc feeding strategies, and we define explicit regions of initial conditions in which the optimal strategy is either the first singular arc strategy or the second strategy.

Keywords. optimal control, minimal time problem, impulsive control, Pontryagin maximum principle, bioreactor.

MSC. 49J15, 49K15, 49N25.

Introduction 1

The operation of a fed-batch bioreactor consists of feeding the reactor with a highly concentrated solution without any removal of liquid before the end. This operating mode presents many advantages over batch or chemostat (continuous culture) operations: a high concentration of cells or products can be obtained, and it allows for the easy control of the operating conditions, in particular the limiting substrate concentration (see [9]). Therefore, fed-batch bioreactors have been widely used in the food and pharmaceutical industries, as well as in wastewater treatment. In a fed-batch process, choosing an adequate feeding strategy is a key feature that can significantly increase productivity. Many authors have proposed feeding strategies using optimal control theory for various types of problems (different bioprocesses and/or objectives, see for example [8] and [10]). In this study, we will focus on the minimal time problem: given initial conditions, the objective is to define a feeding strategy to reach a given substrate concentration in a minimal amount of time with a given maximal volume (representing a completely full tank). The optimal synthesis for this problem has been obtained in [13] using Green's theorem, via the technique introduced in [11], in the following cases:

- For increasing growth functions (e.g., the Monod kinetic, see [12, 17]), the optimal solution is of the Bang-Bang type: it consists of filling the reactor up to the maximum volume with the maximum input flow rate and then waiting until the substrate concentration reaches the desired value.
- For nonmonotonic growth functions with one maximum point (e.g., Haldane kinetic, see [1, 17]), the optimal solution is a singular arc strategy, consisting of regulating the substrate concentration at the maximum of the specific growth rate.

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These results, obtained for regular controls in [13], have been recently extended to allow for impulsive controls (corresponding to instantaneous dilutions), in [7], for the following situations :

- for the case of one microbial species with increasing (e.g., Monod) or one maxima (e.g., Haldane) growth functions,
- for the case in which two microbial species compete for the same substrate with two increasing growth functions that satisfy additional assumptions.

Several new methods have also been proposed for the practical implementation of these optimal strategies (see [3]), including alternative approaches such as extremum seeking (see [5]). In this work, we will focus on the problem of fed-batch operation with growth functions having two local maxima. This type of growth function is observed when the bacterial population can grow via two possible metabolic pathways (e.g., each one is related to a different non-limiting substrate). Indeed, for some microbial species, a high substrate concentration can result in the changing of metabolic pathways (see [6]). A growth function having two local maxima can also be obtained when we consider a growth function with one maximum point associated with inhibition by a product. Under some hypotheses, the product concentration can be expressed as a function of the substrate concentration, and the problem can be rewritten as a growth function with two local maxima [2].

In [15], the problem of minimal time control for a growth function with two local maxima has been addressed using a numerical approach. It appears that the singular arcs defined by the two local maxima are two optimal candidates, but to obtain the optimal synthesis is not easy, because none of the previous methods applied for Monod or Haldane growth function are applicable here. Given the numerical results obtained using a regularization method, the authors conjecture that the state space can be divided into two domains in which each arc strategy is optimal. To solve this problem analytically, we allow impulsive control (see [7]). In general, an impulsive control indicates that the input flow rate is allowed to take values $u_m \gg 1$ corresponding to instantaneous dilution. We consider two cases, which depend on whether the strict global maximum of the growth function is the first local maximum (case B) or the second maximum (case A). The problem is reformulated into a planar affine system with two controls (as was done in [13] without impulsive control) introducing a constant M defined by the initial conditions (see Section 2). We then use the Pontryagin maximum principle (see [14]) to derive the necessary conditions on optimal trajectories. Our method relies on the exclusion of extremal trajectories that have a switching point before reaching one of the two singular arcs. We then conclude by considering which singular strategy starting from a given initial condition has the minimal cost. The paper is organized as follows. In Section 2, the problem is stated, and we derive several general properties about extremal trajectories via the Pontryagin maximum principle. In particular, we provide an explicit expression of the switching functions corresponding to the controls (see lemmas 2.3 and 2.4), which is the starting point for comparing both strategies. These expressions allow, in particular, the easy retrieval of a result in [7] on the optimality of the singular arc strategy in the case of one species with a Haldane growth function. The original proof (see [7]) makes use of the characterization of the value function by using the Hamilton-Jacobi equation (a sufficient condition). In Section 3, we prove the general comparison results between extremal trajectories that are valid for cases A and B. Section 4 and 5 are devoted to cases A and B. The following results are obtained:

- Case A, $M \ge 0$: the optimal synthesis is given by theorem 4.1
- Case A, M < 0: the optimal synthesis is obtained under the hypothesis 4.1 (see theorem 4.2).
- Case B, $M \ge 0$: we prove that the first singular arc is optimal (see theorem 5.1).
- Case B, M < 0: we prove that the first singular arc is optimal (theorem 5.2) provided that the hypotheses 5.1 and 5.2 are satisfied.

For $M \ge 0$, our optimal synthesis proves the conjecture proposed in [15] when impulsive control is allowed. It appears that the case M < 0 (which corresponds to a low initial concentration of biomass) is slightly more delicate to handle than the case $M \ge 0$. In case B, M < 0, hypothesis 5.1 is satisfied when M is small. Hypotheses 4.1 and 5.2 have been verified numerically (see Figure 4).

2 Statement of the problem and general results

2.1 Formulation of the problem

In this subsection, we present the model and the optimal control problem. Let us consider the following control system describing a perfectly mixed reactor operated in fed-batch mode with impulsive control (see [7]):

$$\begin{cases} \dot{x} = \left(r\mu(s) - \frac{u}{v}\right)x, \\ \dot{s} = -r\mu(s)x + \frac{u}{v}(s_{in} - s), \\ \dot{v} = u, \end{cases}$$
(2.1)

where x is the concentration of biomass, s is the concentration of substrate, and v is the volume of water (with concentrations x and s) in the tank. We will assume that the growth function μ has two local maxima $s_1 < s_2$ and one local minimum $s_m \in (s_1, s_2)$, see Figure 1. We will consider two cases:

- Case A: $\mu(s_1) < \mu(s_2)$.
- Case B: $\mu(s_1) > \mu(s_2)$.

We also suppose that $\mu''(s_1) \neq 0$, $\mu''(s_2) \neq 0$, and $\mu''(s_m) \neq 0$, and we define $s'_2 \in [s_m, s_2]$ such that $\mu(s'_2) = \mu(s_1)$ in case A, and similarly, $s'_1 \in [s_1, s_m]$ such that $\mu(s'_1) = \mu(s_2)$ in case B.

The set of admissible controls is defined as follows:

$$\mathcal{U} = \{ \mathbf{u} = (r, u) : [0, \infty[\to (\{0, 1\} \times [0, 1]) \setminus \{(0, 0)\} \mid \text{meas.} \}.$$

Here, u is the input flow rate and r represents an impulse control. An instantaneous addition of volume $v_+ - v_-$ (i.e., a jump from volume v_- to volume v_+) is achieved by taking r = 0 on some interval of time $[\tau_-, \tau_+]$ for system (2.1) and any measurable control u satisfying

$$\int_{\tau_{-}}^{\tau_{+}} u(t)dt = v_{+} - v_{-}, \qquad (2.2)$$

see [7] for more details. In particular, there is no uniqueness of u as long as integral (2.2) is equal to $v_+ - v_-$. An addition of volume $v_+ - v_-$ corresponds to a dilution of the substrate and the biomass:

$$s_{+} = \frac{v_{-}}{v_{+}}s_{-} + \left(1 - \frac{v_{-}}{v_{+}}\right)s_{in}, \ x_{+} = \frac{v_{-}}{v_{+}}x_{-},$$

where s_{-} , x_{-} are the concentrations before dilution and s_{+} , x_{+} are the concentrations after dilution. We



Figure 1: Figure left: example of a growth function (corresponding to case A) that is a sum of two Haldane growth functions having two local maxima $s_1 < s_2$, such that $\mu(s_1) < \mu(s_2)$. Figure right: sum of two Haldane growth functions with $\mu(s_1) > \mu(s_2)$ (case B).

denote by ξ a triple $\xi = (x, s, v)$, and let $E = \mathbb{R}^*_+ \times]0, s_{in}[\times]0, v_m] \subset \mathbb{R}^3$ be the domain of state variables x, s, and v. The target is defined as follows:

$$\mathcal{T} = \{ \xi = (x, s, v) \in E \mid 0 \le s \le s_{ref}, \ v = v_m \},\$$

where s_{ref} is a given reference (low) concentration such that $0 < s_{ref} < s_1 < s_2 < s_{in}$, and v_m is the volume of the tank. For $\xi \in E$ and a control $\mathbf{u} \in \mathcal{U}$, let $t_{\xi}(\mathbf{u})$ be the first entry time in \mathcal{T} . In the impulsive framework, the minimum time problem, for an initial condition $\xi_0 \in E$, can be gathered into:

$$\inf_{\mathbf{u}\in\mathcal{U}}\int_{0}^{t_{\xi_{0}}(\mathbf{u})}r(\tau)d\tau, \text{ s.t. } (x(0),s(0),v(0)) = \xi_{0};$$
(2.3)

see [7] for more details on the reparametrization of the minimum time problem with impulsive control. If (x, s, v) is a solution of (2.1), the function $M := v(x + s - s_{in})$ is constant equal to $v_0(x_0 + s_0 - s_{in})$; hence, we have $x = \frac{M}{v} - (s - s_{in})$, and the system can be gathered into a quasi-affine planar system with two inputs:

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

$$(2.4)$$

Remark 2.1. The sign of the constant $M = v_0(x_0 + s_0 - s_{in})$ defined by the initial conditions plays an important role in the synthesis of the optimal feeding strategy. Note that for repeated fed-batch cultures (i.e., at the end of the culture, the reactor is partially drained, and then a new culture begins using the substrate and biomass concentrations reached at the end of the previous culture), one can easily check that M will tend to 0.

We claim that for any $\xi_0 \in E$, the minimum time to reach \mathcal{T} is finite. Indeed, one can reach volume v_m from any $\xi_0 \in E$ by an impulse of volume $v_m - v_0$ (that is, r = 0). If the concentration of substrate is greater than s_{ref} , we put u = 0 and r = 1 until $s(t) \leq s_{ref}$. This strategy steers any $\xi_0 \in E$ to the target \mathcal{T} in finite time, which proves that (2.3) is finite. The existence of an optimal solution of (2.3) is not guaranteed by Filipov's theorem (see [4]), as the set of admissible controls is not convex (recall that $r(\cdot) \in \{0, 1\}$). Let us now consider the *relaxed problem*, that is, the problem (2.3) in which the control (r, u) is allowed to take values within $U := [0, 1] \times [0, 1]$. By the convexity of U and the cost functional, the existence of an optimal control for the relaxed problem is standard by Filipov's theorem, see [4]. Without loss of generality, we may consider trajectories such that $(r, u) \neq 0$ (if r = u = 0, the cost is unchanged while the dynamics are stationary). We will see in the next section that an optimal control of the relaxed problem can be taken such that $r(\cdot) \in \{0, 1\}$.

2.2 Pontryagin maximum principle

In this subsection, we derive the necessary conditions for an optimal control by the Pontryagin maximum principle (PMP), and we compute the singular arcs. We also prove the existence of an optimal solution of problem (2.3). Let γ_0 be the curve, in the plane s - v, defined by:

$$\gamma_0(s) = v_m \left(\frac{s_{in} - s_{ref}}{s_{in} - s}\right), \ s \in [0, s_{ref}].$$

$$(2.5)$$

In the rest of the paper, we will consider initial conditions for the system (2.4) in the set \mathcal{D} defined as follows:

$$\mathcal{D} = \left\{ (s_0, v_0) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \mid s_0 \in (0, s_{in}), \ 0 < v_0 < \min(\gamma_0(s_0), v_m), \ M + v_0(s_{in} - s) > 0 \right\}.$$
 (2.6)

Note that the last condition guarantees that the initial conditions ξ_0 of system (2.1) satisfy $x_0 > 0$. We will prove in the next subsection that for initial conditions (s_0, v_0) such that $\gamma_0(s_0) \le v_0 \le v_m$, the optimal control is a single impulse from volume v_0 to volume v_m (see proposition 2.3). Therefore, we will assume throughout the paper that initial conditions are in \mathcal{D} . The Hamiltonian of the system $H = H(s, v, \lambda_s, \lambda_v, \lambda_0, r, u)$ is:

$$H = -r\lambda_s \mu(s) \left(\frac{M}{v} - (s - s_{in})\right) + u \left(\frac{\lambda_s(s_{in} - s)}{v} + \lambda_v\right) + \lambda_0 r.$$
(2.7)

Let us apply the Pontryagin maximum principle to the relaxed problem. Let (r, u) be an optimal solution and (s, v) the corresponding solution of (2.4). Then, there exists $t_f > 0$, $\lambda_0 \leq 0$ and an absolutely continuous map $\lambda = (\lambda_s, \lambda_v) : [0, t_f] \to \mathbb{R}^2$ 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:

$$\begin{cases} \dot{\lambda}_s = \lambda_s (r\mu'(s)x - r\mu(s) + \frac{u}{v}), \\ \dot{\lambda}_v = \frac{\lambda_s}{v^2} (-r\mu(s)M + u(s_{in} - s)), \end{cases}$$
(2.8)

and we have the maximality condition:

for a.e.
$$t \in [0, t_f], \ H(s(t), v(t), \lambda_s(t), \lambda_v(t), \lambda_0, r(t), u(t)) = \max_{(\tilde{r}, \tilde{u}) \in U} H(s(t), v(t), \lambda_s(t), \lambda_v(t), \lambda_0, \tilde{r}, \tilde{u}) = 0.$$

(2.9)

The Hamiltonian in (2.9) is zero, as t_f is free. Without loss of generality, we may assume $\lambda_0 = -1$. Next, define the *switching functions* ϕ_1 and ϕ_2 associated with controls r and u:

$$\begin{cases} \phi_1(t) = -\lambda_s \mu(s) \left(\frac{M}{v} - (s - s_{in})\right) - 1, \\ \phi_2(t) = \lambda_s \frac{s_{in} - s}{v} + \lambda_v. \end{cases}$$
(2.10)

We call an *extremal trajectory* a quintuplet $(s(\cdot), v(\cdot), \lambda_s(\cdot), \lambda_v(\cdot), r(\cdot), u(\cdot))$ satisfying (2.4)-(2.8)-(2.9). It follows that any extremal trajectory satisfies for a.e. $t \in [0, t_f]$:

$$r(t)\phi_1(t) + u(t)\phi_2(t) = 0.$$
(2.11)

We obtain from (2.9) that any optimal control satisfies the following control law: for a.e. $t \in [0, t_f]$, we have

$$\begin{cases} \phi_1(t) < 0, \ \phi_2(t) = 0 \implies r(t) = 0, \ u(t) \in (0, 1], \\ \phi_2(t) < 0, \ \phi_1(t) = 0 \implies u(t) = 0, \ r(t) \in (0, 1], \\ \phi_1(t) = 0, \ \phi_2(t) = 0 \implies r(t) \in (0, 1], \ u(t) \in (0, 1] \end{cases}$$
(Singular arc). (2.12)

In particular, an extremal trajectory has a singular arc on some time interval I if both switching functions satisfy $\phi_1(t) = \phi_2(t) = 0$ for all $t \in I$. Derivating the switching functions yields:

$$\dot{\phi}_1(t) = -u\phi(t), \ \dot{\phi}_2(t) = r\phi(t),$$
(2.13)

where:

$$\phi(t) = \frac{\lambda_s \mu'(s)(s_{in} - s)x}{v}.$$
(2.14)

The next lemma will be useful in the following.

Lemma 2.1. If (s_0, v_0) is in \mathcal{D} , then any optimal trajectory satisfies $\lambda_s < 0$.

Proof. An optimal trajectory is a concatenation of arcs where u = 0 (no feeding), r = 0 (impulse), or s is constant with $s \in \{s_1, s_2, s_m\}$ (singular arc, see lemma 2.2 (i)). If the initial condition is in \mathcal{D} , any optimal trajectory contains an arc u = 0 (otherwise, the trajectory would not reach \mathcal{T}). If λ_s vanishes at some point $t_0 \in [0, t_f]$, then $\lambda_s \equiv 0$ from (2.8). Hence, when u = 0, we obtain from (2.7) that r = 0, which is not possible (recall that we assumed $(r, u) \neq (0, 0)$). Hence, λ_s is always non-zero and of constant sign. Moreover, when u = 0, one has from (2.7) $-r\lambda_s\mu(s)x - r = 0$; thus, $\lambda_s < 0$.

From the expression of ϕ and the sign of λ_s , one can prove the following proposition that will be useful to perform the optimal synthesis in the two next sections.

Proposition 2.1. (i). Let $(s_0, v_0) \in \mathcal{D}$ such that $s_0 \in (s_m, s_2]$ and let us consider an extremal trajectory satisfying u = 0 at time 0. Then, there exists $t_1 > 0$ with $s(t_1) < s_m$ such that we have u = 0 on $[0, t_1]$. (ii). Let $(s_0, v_0) \in \mathcal{D}$ such that $s_0 \in [s_1, s_m)$, $v_0 < v_m$, and let us consider an extremal trajectory satisfying r = 0 at time 0. Then, there exists $t'_1 > 0$ with $s(t'_1) > s_m$ such that we have r = 0 on $[0, t'_1]$.

Proof. Let us prove (i). From (2.14), we have that ϕ is non-negative when $s(t) \in [s_1, s_m]$, and ϕ is negative when $s(t) \in [s_m, s_2]$. It follows that if $s(t) \in [s_1, s_m]$, then ϕ_2 is increasing, whereas if $s(t) \in [s_m, s_2]$, then ϕ_2 is decreasing. When u = 0, the concentration of substrate s(t) is strictly decreasing at time 0; thus, ϕ_2 remains negative until $s(t) = s_m$. If ϕ_u is always negative, then the trajectory does not reach the target (as $v_0 < v_m$). Therefore, there exists $t_1 > 0$ with $s(t_1) < s_m$ such that $\phi_2(t_1) = 0$. The proof of (ii) is similar using $\phi_1(0) \leq 0$ and the monotonicity of ϕ_1 for $s(t) \in [s_1, s_m]$.

In general, the previous lemma means that an arc r = 0 (resp. an arc u = 0) starting with $s_0 \in [s_1, s_m)$ (resp. $s_0 \in (s_m, s_2]$) always passes though the line $s = s_m$. Let us now evaluate a singular arc strategy.

Lemma 2.2. Let us consider a trajectory that contains a singular arc on some time interval $[t_0, t_1]$. Then: (i). The concentration of substrate is constant on $[t_0, t_1]$, and $s \in \{s_1, s_2, s_m\}$.

(ii). If the singular arc is optimal, then $s \in \{s_1, s_2\}$.

(iii). The cost of a singular arc from a volume v_0 to a volume v_1 is:

$$\int_{t_0}^{t_1} r(t)dt = \frac{1}{\mu(s_i)} \ln\left(\frac{M + v_1(s_{in} - s_i)}{M + v_0(s_{in} - s_i)}\right), \ i = 1, 2,$$
(2.15)

and the singular control can be expressed as follows:

$$u_{s_i} = \mu(s_i) \left(v + \frac{M}{s_{in} - s_i} \right), \ i = 1, 2.$$
(2.16)

Proof. By the definition of a singular arc, we have $\phi_1(t) = \phi_2(t) = 0$ on $[t_0, t_1]$. By derivating, we obtain $\phi(t) = 0$ for $t \in [t_0, t_1]$ as $(r, u) \neq (0, 0)$. In view of (2.14), the only possibility for ϕ to be zero on $[t_0, t_1]$ is $\mu'(s) = 0$; hence, s must be constant on the interval $[t_0, t_1]$, that is, $s = s_1$, $s = s_m$ or $s = s_2$, which proves (i). By using $\dot{s} = 0$ on $[t_0, t_1]$, (2.4) becomes:

$$\dot{v} - r\mu(s)v = r\mu(s)\frac{M}{s_{in} - s}$$

Solving this equation yields:

$$v_1 = \left(v_0 + \frac{M}{s_{in} - s}\right) e^{\mu(s) \int_{t_0}^t r(\tau) d\tau} - \frac{M}{s_{in} - s},$$

and we obtain (2.15). By derivating, we obtain (2.16), which proves (iii). From (2.15), we may assume that r = 1 along a singular arc. Indeed, it is enough to ensure that the L^1 -norm of r on some time interval (where the volume goes from v_0 to v_1) is equal to the right hand side of (2.15).

Let us now discuss the optimality of a singular arc. By derivating $\phi(t)$ and replacing r(t) by 1, we obtain:

$$\phi'(t) = \frac{\lambda_s x}{v} \left(\mu''(s)(s_{in} - s)(-\mu(s)x + \frac{u}{v}(s_{in} - s)) + x\mu(s)\mu'(s) - 2\frac{u}{v}\mu'(s)(s_{in} - s) + \mu'(s)x \right).$$
(2.17)

An optimal control u must satisfy the Legendre-Clebsch necessary condition along the trajectory, that is, $\frac{\partial}{\partial u} \frac{d^2}{dt^2} H_u \ge 0$, see e.g., [16]. Combining $\mu'(s) = 0$ and (2.17) yields:

$$\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u = \mu''(s)\frac{\lambda_s x(s_{in}-s)^2}{v};$$

Thus, one must have $\mu''(s) \leq 0$ (recall that $\lambda_s < 0$). Hence, the only possibility for s is $s = s_1$ or $s = s_2$, which proves (ii).

Theorem 2.1. There exists an optimal solution of (2.3) such that $r \in \{0, 1\}$.

Proof. Let $(r, u) \neq (0, 0)$ an optimal solution of the relaxed problem. Notice that (r, u) satisfies (2.12) for a.e. $t \in [0, t_f]$. In the case of an impulse, we have r = 0, whereas in the case of a singular arc, one can take r = 1 by the previous lemma. Let us now examine the case where u = 0 (no feeding). If u = 0 on some time interval $[t_0, t_1]$, the volume v is constant, and we have $\dot{s} = r(t)f(s(t))$, where $f(s) = -\mu(s)(M/v - (s - s_{in}))$. Let us put

$$\begin{cases} \theta = \int_{t_0}^t r(\tau) d\tau, \\ z(\theta(t)) = s(t). \end{cases}$$

By derivating, one has $\frac{dz}{d\theta}(\theta(t))r(t) = \dot{s}(t) = r(t)f(s(t))$; thus, we have:

$$\frac{dz}{d\theta} = f(z(\theta)), \tag{2.18}$$

as r is non-zero. Moreover, z satisfies $z(0) = s(t_0)$ and $z(\overline{\theta}) = s(t_1)$, where $\overline{\theta} = \int_{t_0}^{t_1} r(\tau) d\tau$, and the cost remains unchanged (as the cost of z on the interval $[0,\overline{\theta}]$ is $\overline{\theta}$). We can repeat this argument on any arc u = 0 of the trajectory, which allows us to take r = 1 by (2.18). This concludes the proof.

Remark 2.2. Theorem 2.1 answers a question raised in [7] on the existence of an optimal solution of (2.3) with $r \in \{0, 1\}$ in the case of one species. The existence of an optimal control of (2.3) with a control r such that $r \in \{0, 1\}$ remains an open question in presence of more than one species.

Definition 2.1. The singular arc strategy SAS_i , i = 1, 2 (corresponding to $s = s_1$ or $s = s_2$) starting at some point $(s_0, v_0) \in D$ is defined as follows:

$$(r(s_0, v_0), u(s_0, v_0)) = \begin{cases} (1, u_{s_i}) \text{ if } s_0 = s_i \text{ and } v_0 < v_m, \\ (1, 0) \text{ if } s > s_i \text{ or } v_0 = v_m, \\ (0, \tilde{u}) \text{ if } s < s_i \text{ and } v_0 < v_m, \end{cases}$$

where control \tilde{u} is any measurable function taking values in [0, 1] such that (2.2) holds in presence of a dilution.

The next proposition is concerned with some restrictions on the parameters of the system in order to obtain admissible singular arcs.

Proposition 2.2. (i). If M < 0 and $\mu(s_i)v_m \leq 1$ for i = 1, 2 then both singular strategies are well-defined. (ii). If $M \geq 0$ and $\mu(s_i)\left(v_m + \frac{M}{s_{in} - s_i}\right) \leq 1$, i = 1, 2, then both singular strategies are well-defined.

Proof. By lemma 2.2, with i = 1, 2, the control u_{s_i} is admissible if and only if:

$$0 \le \mu(s_i) \left(v(t) + \frac{M}{s_{in} - s_i} \right) \le 1, \ t \in [t_0, t_1].$$
(2.19)

As $\{(s_0, v_0) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ | s_0 \in (0, s_{in}), 0 < v_0 \leq v_m, M + v_0(s_{in} - s) > 0\}$ is invariant by the dynamics, and the left inequality in (2.19) is always satisfied. When M < 0, a sufficient condition to have an admissible control is $\mu(s_i)v_m \leq 1, i = 1, 2$ (to ensure the right inequality of (2.19)). This proves (i). The proof of (ii) is similar.

Remark 2.3. From a practical point of view, we assume that the parameters of the system always satisfy the conditions given by the previous proposition.

2.3 Computations of the switching functions

In this subsection, we compute the switching functions in the case of non-feeding (that is u = 0 and r = 1) and in the case of an impulse (r = 0) in order to address the global optimality of the singular arc strategies SAS_i , i = 1, 2 in the next section. Let us define a function ψ_v by:

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

Notice that ψ_v is non-negative by (2.4). In the case where M = 0, one has $\psi_v(s) = \frac{1}{v}$. Moreover, one has $\psi'_v(s) = \frac{-M}{(M+v(s_{in}-s))^2}$; hence, if M < 0, then ψ_v is increasing, whereas if M > 0, then ψ_v is decreasing.

Lemma 2.3. Let us consider an extremal trajectory starting at $(s_0, v_0) \in \mathcal{D}$ at time 0 with u = 0 on some time interval $[0, t_1]$. Then, we have for $t \in [0, t_1]$:

$$\lambda_s(t) = \frac{-v_0}{\mu(s(t))(M + v_0(s_{in} - s(t)))}, \ \lambda_v(t) = \lambda_v(0) + \int_{s_0}^{s(t)} \frac{\psi'_{v_0}(s)}{\mu(s)} ds,$$
(2.20)

$$\phi_2(t) = \lambda_v(0) - \frac{\psi_{v_0}(s_0)}{\mu(s_0)} + \int_{s_0}^{s(t)} \psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds.$$
(2.21)

The cost associated to this trajectory is:

$$J = -\int_{s_0}^{s(t_1)} \frac{ds}{\mu(s)\left(\frac{M}{v_0} + s_{in} - s\right)}$$
(2.22)

Proof. The expression of λ_s is straightforward from the expression of the Hamiltonian along u = 0. We then obtain $\dot{\lambda}_v = \frac{\frac{M}{v_0}}{M + v_0(s_{in} - s)}$. By dividing by \dot{s} (which is non-zero as $(r, u) \neq (0, 0)$), we obtain:

$$\frac{d\lambda_v}{ds} = -\frac{M}{\mu(s)(M + v_0(s_{in} - s))^2} = \frac{\psi_{v_0}'(s)}{\mu(s)}$$

and we obtain the desired expression of λ_v by integrating. Replacing λ_s into the expression of ϕ yields:

$$\phi_2(t) = \lambda_v(t) - \frac{\psi_{v_0}(s(t))}{\mu(s(t))},$$

and we obtain the desired expression for ϕ_2 by integrating by parts the expression of λ_v . Finally, the cost J is obtained by integrating the differential equation \dot{s} along u = 0.

Let $\mathcal{D}' = \{(s_0, v_0) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \mid \gamma_0(s_0) \leq v_0 \leq v_m\}$. From the previous lemma, we obtain the optimal solution for any initial conditions in \mathcal{D}' .

Proposition 2.3. (i). If $(s_0, v_0) \in \mathcal{D}'$, then the optimal feedback steering (s_0, v_0) to the target is an impulse of volume $v_m - v_0$.

(ii). An extremal trajectory starting at some point $(s_0, v_0) \in \mathcal{D}$ such that $s_0 \leq s_1, v_0 < v_m$ and satisfying u = 0 on a time interval $[0, t_1]$ is not optimal.

Proof. (i). If $v_0 = v_m$, then the initial point is in \mathcal{T} , and the result is proved. Assume $v_0 < v_m$. If an optimal trajectory satisfies u = 0 with volume $v < v_m$ on some time interval $[t_0, t_1]$, we must have $\phi_2(t_0) \leq 0$, and there exists a time $t'_0 > 0$ such that $\phi_2(t'_0) = 0$ (otherwise, the trajectory would not reach \mathcal{T}). We obtain:

$$\phi_2(t_0) < \phi_2(t'_0) = 0 = \phi_2(t_0) + \int_{s(t_0)}^{s(t'_0)} \psi_v(s) \frac{\mu'(s)}{\mu^2(s)} ds;$$

hence, we obtain:

$$\int_{s(t_0)}^{s(t_0')} \psi_v(s) \frac{\mu'(s)}{\mu^2(s)} ds > 0.$$

But one has $\psi_v(s) > 0$, $\mu'(s) > 0$ (recall that $s < s_1$), and $s(t_0) > s(t'_0)$. Consequently, the integral above is negative, which is a contradiction. We can use the same argument for proving (ii).

Corollary 2.1. Consider an optimal trajectory starting from a point $(s_0, v_0) \in \mathcal{D}$ such that $0 < s_0 \leq s_2$ and $0 < v_0 < v_m$. Assume that u = 0 in the neighborhood of zero.

(i). There exists a time t_0 such that $\phi_2(t_0) = 0$, $s(t_0) < s_m$, and we have:

$$\int_{s(t_0)}^{s_0} \psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds < 0 \tag{2.23}$$

(ii). Moreover, if $M \leq 0$, we have:

$$\mu(s(t_0)) > \mu(s_0). \tag{2.24}$$

Proof. We have $\phi_2(0) < 0$; hence, ϕ_2 remains negative for t close to zero. As $v_0 < v_m$, the switching function must be zero at a certain time, and we obtain the existence of a time t_0 such that $\phi_2(t_0) = 0$. Notice that $s(t_0) < s_m$. Indeed, if $s_0 < s_m$, the result is clear, as s is decreasing along u = 0. If $s_0 > s_m$, the result follows from proposition 2.1. The previous conditions on the switching function can be written:

$$\phi_2(0) < 0 = \phi_2(t_0) = \phi_2(0) + \int_{s(t_0)}^{s_0} -\psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds = 0,$$

hence:

$$\int_{s(t_0)}^{s_0} -\psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds > 0,$$

which proves (i). From this last inequality, we obtain:

$$\int_{s_m}^{s_0} \psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds < \int_{s(t_0)}^{s_m} \psi_{v_0}(s) \frac{-\mu'(s)}{\mu^2(s)} ds.$$
(2.25)

When $M \leq 0$, ψ_{v_0} is increasing; therefore:

$$\psi_{v_0}(s_m) \int_{s_m}^{s_0} \frac{\mu'(s)}{\mu^2(s)} ds \le \int_{s_m}^{s_0} \psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds < \int_{s(t_0)}^{s_m} \psi_{v_0}(s) \frac{-\mu'(s)}{\mu^2(s)} ds \le \psi_{v_0}(s_m) \int_{s(t_0)}^{s_m} \frac{-\mu'(s)}{\mu^2(s)} ds.$$

We obtain the inequality:

 $\psi_{v_0}(s_m)\left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s_0)}\right) < \psi_{v_0}(s_m)\left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s(t_0))}\right),$

which gives (2.24).

We now compute the switching functions in the case of an impulse.

Lemma 2.4. Assume that an extremal trajectory starting at $(s_0, v_0) \in \mathcal{D}$ with $0 < v_0 < v_m$ satisfies r = 0 on $[0, t_0]$. Then, one has:

$$\lambda_s(t) = \frac{\lambda_s(0)}{v_0} v(t), \ \lambda_v(t) = \lambda_v(0) + \frac{\lambda_s(0)}{v_0} (s - s_0),$$
(2.26)

$$\phi_1(t) = -\lambda_s(0)x_0\mu(s) - 1, \ \phi_2(t) = \lambda_v(0) + \frac{\lambda_s(0)(s_{in} - s_0)}{v_0} = 0.$$
(2.27)

Proof. The proof is straightforward from the state-adjoint equation and the Hamiltonian. Notice that the adjoint vector must satisfy $\lambda_v(0) + \frac{\lambda_s(0)(s_{in}-s_0)}{v_0} = 0$ to ensure $\phi_2 = 0$ along the impulse.

Remark 2.4. The cost associated to this trajectory is null.

Lemma 2.5. Assume that an extremal trajectory starting at $(s_0, v_0) \in \mathcal{D}$ with $0 < v_0 < v_m$ satisfies r = 0 on $[0, t_0]$ and $\phi_1(t_0) = 0$ for $t_0 > 0$. Then, one has:

$$\mu(s(t_0)) \ge \mu(s_0). \tag{2.28}$$

Proof. Condition $\phi_1(0) \le 0$ gives $\mu(s_0) \le \frac{1}{-\lambda_s(0)x_0}$, and condition $\phi_1(t_0) = 0$ gives $-\lambda_s(0)x_0\mu(s(t_0)) - 1 = 0$; hence, $\mu(s(t_0)) = \frac{1}{-\lambda_s(0)x_0} \ge \mu(s_0)$.

The previous lemma has simple consequences:

- In case A, any trajectory starting at $s_0 \ge s_2$ with an impulse is not optimal, as μ is strictly decreasing on $[s_2, +\infty)$. This remark (combined with proposition 2.3 (ii)) allows us to retrieve the optimality of a singular strategy for one species and a Haldane growth function in the impulsive case, see [7] (the proof in [7] makes use of the value function and the Hamilton-Jacobi equation).
- In case A, any extremal trajectory starting at $(s_0, v_0) \in \mathcal{D}$, $s_0 \in [s_1, s_m]$ with an impulse, is such that ϕ_1 will vanish between s'_0 and $\min(s_2, s^*(s_0, v_0))$ where $s'_0 \in [s_m, s_2]$ satisfies $\mu(s'_0) = \mu(s_0)$ and $s^*(s_0, v_0)$ is defined by $s^*(s_0, v_0) = s_0 \frac{v_0}{v_m} + (1 \frac{v_0}{v_m})s_{in}$. Indeed, combining lemma 2.5 and the monotonicity of μ on $[s_2, +\infty)$, we have that an extremal trajectory crossing $s = s_2$ with an impulse is not optimal.
- In case B, any trajectory starting at $s_1 \leq s_0 < s'_1$ with an impulse is not optimal by using (2.28).

3 General comparison results for case A and B

In this section, we compare the cost of several extremal trajectories in order to exclude some candidates for optimality. Let us define:

$$s_1^* = \begin{cases} s_1 & \text{for case A}, \\ s_1' & \text{for case B}, \end{cases}$$
 and $s_2^* = \begin{cases} s_2' & \text{for case A}, \\ s_2 & \text{for case B}, \end{cases}$

and let $\gamma_2^*(s)$, $\gamma_2(s)$, such that:

$$\gamma_2^*(s) = v_m \left(\frac{s_{in} - s_2^*}{s_{in} - s}\right), \ \gamma_2(s) = v_m \left(\frac{s_{in} - s_2}{s_{in} - s}\right)$$

Notice that for $s \in]0, s_2[:$

$$\gamma_2(s) < \gamma_2^*(s)$$
 for case A, and $\gamma_2(s) = \gamma_2^*(s)$ for case B.

Let us now consider C_2 and C_2^* defined by:

$$\mathcal{C}_2 = \{(s,v) \in (0,s_2] \times (0,v_m] \mid v = \gamma_2(s)\}, \ \mathcal{C}_2^* = \{(s,v) \in (0,s_2] \times (0,v_m] \mid v = \gamma_2^*(s)\}.$$

The curves C_2 and C_2^* are *dilution curves*. This result indicates that if $(s_0, v_0) \in C_2$, then an impulse of volume $v - v_0$ (with $v < v_m$) transforms (s_0, v_0) into another point of C_2 . It is important to see that any set

$$F_{\overline{s}} := \left\{ (s, v) \in (0, s_{in}) \times (0, v_m) \mid v \ge v_m \left(\frac{s_{in} - \overline{s}}{s_{in} - s} \right) \right\}$$

where $\overline{s} \in (0, s_{in})$, is such that any extremal trajectory starting in $F_{\overline{s}}$ will stay in this set for all t. In the following, we make use of the notations:

- $I_{s_-,v_-}^{s_+,v_+}$ denotes a dilution (or impulse) from (s_-,v_-) to (s_+,v_+) achieved by r=0 and any admissible control u such that $\int_{\tau_-}^{\tau_+} u(\tau) d\tau = v_+ v_-$. For short, we will also make use of the notation I to denote an impulse.
- $NF_{s_0,v_0}^{s'_0,v_0}$ denotes an arc u = 0 (no feeding) at constant volume v_0 from a concentration s_0 to a concentration $s'_0 < s_0$. For short, we will also make use of the notation NF to denote an arc u = 0.
- $SA_i^{v_1,v_2}$ denotes a singular arc s_i from volume v_1 to volume v_2 , i = 1, 2.

We will say that an extremal trajectory has a switching (or switching point) at some time t_0 if it contains a sequence $I_{s_-,v_-}^{s_+,v_+} NF_{s_+,v_+}^{\overline{s},v_+}$ (with $s_+ > s_-$, $\overline{s} < s_+$) or $NF_{s_0,v_0}^{s_0',v_0}I_{s_0',v_0}^{s_+,v_+}$ (with $s_0' < s_0$, $s_+ > s_0'$) such that the control (r, u) is non-constant in a neighborhood of t_0 . We now examine the possibility for an optimal control to have switching points at some point (s, v) with $v < v_m$ and $s \in]s_1, s_2^*[$, i = 1, 2. In the next lemma, we prove that for certain initial conditions, a trajectory reaching the singular arc s_2 with one switching point is not optimal. The proof of this lemma is illustrated on Figure 2.

Lemma 3.1. Let $(s_0, v_0) \in \mathcal{D}$ be a point such that $s_1^* < s_0 < s_2$. A sequence $NF_{s_0, v_0}^{s_-, v_0}I_{s_-, v_0}^{s_2, v_+}$ with $s_- > s_1^*$, and $v_0 < \gamma_2(s_-)$ is not optimal.

Proof. The cost of the sequence above is:

$$J_1 = \int_{s_-}^{s_0} \frac{ds}{\mu(s)(\frac{M}{v_0} + s_{in} - s)}$$

and we have by definition of the dilution $s_2 = \frac{v_0}{v_+}s_- + \left(1 - \frac{v_0}{v_+}\right)s_{in}$. As $\mu(s) \le \mu(s_2)$, we obtain

$$J_1 \ge \frac{1}{\mu(s_2)} \int_{s_-}^{s_0} \frac{ds}{\frac{M}{v_0} + s_{in} - s} = \frac{1}{\mu(s_2)} \ln\left(\frac{M + v_0(s_{in} - s_-)}{M + v_0(s_{in} - s_0)}\right)$$

The cost of the sequence $I_{s_0,v_0}^{s_2,v_2}SA_2^{v_2,v_+}$ is:

$$J_2 = \frac{1}{\mu(s_2)} \ln \left(\frac{M + v_+(s_{in} - s_2)}{M + v_2(s_{in} - s_2)} \right),$$

where we have $s_2 = \frac{v_0}{v_2} s_0 + \left(1 - \frac{v_0}{v_2}\right) s_{in}$. Using $\frac{v_0}{v_2} = \frac{s_{in} - s_2}{s_{in} - s_0}$, $\frac{v_0}{v_+} = \frac{s_{in} - s_2}{s_{in} - s_-}$, we obtain:

$$J_1 - J_2 \ge \frac{1}{\mu(s_2)} \left(\ln \left(\frac{M + v_0(s_{in} - s_-)}{M + v_0(s_{in} - s_0)} \right) - \ln \left(\frac{M + v_+(s_{in} - s_2)}{M + v_2(s_{in} - s_2)} \right) \right) = 0,$$

lemma.

which proves the lemma.

Corollary 3.1. Any trajectory (s(t), v(t)) starting at some point $(s_0, v_0) \in \mathcal{D}$ with $s_1^* \leq s_0 < s_2$, $v_0 < v_m$, such that $s(t) \geq s_1^*$ for all t and containing a sequence $NF_{s_b, v_b}^{s_c, v_b} I_{s_c, v_b}^{s_2, v_c}$, is not optimal.

Proof. It is enough to compare the trajectory with the one that coincides until the point (s_b, v_b) and contains the sequence $I_{s_b,v_b}^{s_2,v_+}SA_2^{v_+,v_c}$. By lemma 3.1, this trajectory has a lower cost than the initial one, which concludes the proof.



Figure 2: *Figure left*: illustration of the proof of lemma 3.1 for case B. *Figure right*: illustration of the proof of lemma 5.1 for case A.

Lemma 3.2. Let $(s_0, v_0) \in \mathcal{D}$ be a point such that $v_0 < v_m$, $s_0 > s_1$. Then, any extremal trajectory that contains a sequence $NF_{s_0,v_0}^{s_-,v_0}I_{s_-,v_0}^{s^+,v_+}NF_{s_+,v_+}^{s_1,v_+}$ with $s_1 < s_- < s_0$ and $s_+ \leq s_2$ is not optimal.

Proof. Let $t_{s_-} < t_{s_+}$ the two instants in which the sequence contains a switch. If the trajectory is optimal, we must have $\mu(s_-) = \mu(s_+)$ given that $\phi_1(t_{s_-}) = \phi_1(t_{s_+}) = 0$ (see lemmas 2.4 and 2.5). Consequently, one has $s_- < s_m < s_+$. Now, let us choose an $\varepsilon > 0$ small enough such that $s_- - \varepsilon > s_1$ and $s_+ - \varepsilon' > s_m$ with $\varepsilon' = \frac{v_+}{v_0}\varepsilon$. We will show that the cost J_1^{ε} of the sequence $NF_{s_0,v_0}^{s_--\varepsilon,v_0}I_{s_--\varepsilon,v_0}^{s^+-\varepsilon',v_+}NF_{s_+-\varepsilon',v_+}^{s_1,v_+}$ is lower than the cost J_2 of the sequence $NF_{s_0,v_0}^{s_-,v_0}NF_{s_+,v_+}^{s_1,v_+}$. Indeed, we have $\mu(s) \leq \mu(s_+)$ for $s \in [s^+ - \varepsilon', s_+]$ and $\mu(s) \geq \mu(s_-)$ for $s \in [s_- - \varepsilon, s_-]$ so that:

$$J_{2} - J_{1}^{\varepsilon} = \int_{s_{+}-\varepsilon'}^{s_{+}} \frac{ds}{\mu(s)(\frac{M}{v_{+}} + s_{in} - s)} - \int_{s_{-}-\varepsilon}^{s_{-}} \frac{ds}{\mu(s)(\frac{M}{v_{0}} + s_{in} - s)}$$

$$> \frac{1}{\mu(s_{+})} \int_{s_{+}-\varepsilon'}^{s_{+}} \frac{ds}{\frac{M}{v_{+}} + s_{in} - s} - \frac{1}{\mu(s_{-})} \int_{s_{-}-\varepsilon}^{s_{-}} \frac{ds}{\frac{M}{v_{0}} + s_{in} - s}$$

$$> \frac{1}{\mu(s_{+})} \ln\left(\frac{M + v_{+}(s_{in} - s_{+} + \varepsilon')}{M + v_{+}(s_{in} - s_{+})}\right) - \frac{1}{\mu(s_{-})} \ln\left(\frac{M + v_{0}(s_{in} - s_{-} + \varepsilon)}{M + v_{0}(s_{in} - s_{-})}\right).$$

Moreover, the dilution can be written:

$$\frac{v_0}{v_+} = \frac{s_{in} - s_+}{s_{in} - s_-} = \frac{s_{in} - s_+ + \varepsilon'}{s_{in} - s_- + \varepsilon}.$$

As $\mu(s_{-}) = \mu(s_{+})$, we obtain $J_2 - J_1^{\varepsilon} > 0$, which concludes the proof.

In the following, we will focus on trajectories containing a sequence NF SA_1 . Let us recall that along an arc u = 0 starting at some point $(s_0, v_0) \in \mathcal{D}$, the switching function ϕ_2 can be expressed by:

$$\phi_2(t) = \phi_2(0) + \int_{s_0}^{s(t)} \psi_{v_0}(s) \frac{\mu'(s)}{\mu^2(s)} ds, \qquad (3.1)$$

and let us define a function F by:

$$(s,v) \in \mathcal{D} \longmapsto F(s,v) = \int_{s_1}^s \psi_v(\sigma) \frac{\mu'(\sigma)}{\mu^2(\sigma)} d\sigma$$
(3.2)

It follows that if $\phi_2 < 0$ until a time t_{s_1} such that $s(t_{s_1}) = s_1$, then we have $\phi_2(t_{s_1}) = \phi_2(0) - F(s_0, v_0)$. We will see in the following sections that the sign of the function F(s, v) is of particular interest.

Lemma 3.3. We have $F(s_m, v) < 0$ for any volume v, and for given $v, s \mapsto F(s, v)$ is increasing with respect to s in the interval (s_m, s_2) . Moreover, for case A, we have: (i). If M > 0, then $F(s'_2, v) < 0$. (ii). If M = 0, then $F(s'_2, v) = 0$.

(iii). If M < 0, then $F(s'_2, v) > 0$.

Proof. First, $\psi_v(s)\frac{\mu'(s)}{\mu^2(s)}$ is negative for $s \in (s_1, s_m)$ and positive for $s \in (s_m, s_2)$, which proves that $F(s_m, v) < 0$ and that $s \mapsto F(s, v)$ is increasing with respect to s in the interval (s_m, s_2) . Let us prove (i). Assume that the inequality does not hold. Then, we have:

$$\int_{s_1}^{s_m} \psi_v(s) \frac{\mu'(s)}{\mu^2(s)} ds + \int_{s_m}^{s_2'} \psi_v(s) \frac{\mu'(s)}{\mu^2(s)} ds \ge 0,$$

that is:

$$I_1 := \int_{s_1}^{s_m} \psi_v(s) \left(-\frac{\mu'(s)}{\mu^2(s)} \right) ds \le \int_{s_m}^{s'_2} \psi_v(s) \frac{\mu'(s)}{\mu^2(s)} ds := I_2$$

Using that ψ_v is decreasing on $[s_1, s_2]$, and $\mu(s'_2) = \mu(s_1)$, we obtain

$$\psi_v(s_m) \left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s_1)}\right) < I_1 \le I_2 < \psi_v(s_m) \left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s_1)}\right),$$

which is a contradiction. The proof of (iii) is analogous, given that $\psi_v(s)$ is increasing with M < 0. To prove (ii), notice that $s \mapsto \psi_v(s)$ is constant, so that $F(s'_2, v) = 0$ by (3.2).

Remark 3.1. For case A, one can prove more generally that if $s \mapsto \alpha(s)$ is a non-decreasing function (resp. $s \mapsto \beta(s)$ is a non-increasing function), then $\int_{s_1}^{s'_2} \alpha(s) \frac{\mu'(s)}{\mu^2(s)} ds \ge 0$ (resp. $\int_{s_1}^{s'_2} \beta(s) \frac{\mu'(s)}{\mu^2(s)} ds \le 0$).

4 Optimal synthesis for case A

In this section, we study the optimality of the singular arcs s_1 and s_2 in case A.

4.1 Preliminary results for all M

In the next proposition, we prove that if a trajectory satisfies $s(t_0) = s_1$ for a certain time t_0 , then it is optimal to stay on the first singular arc until the tank is completely filled.

Proposition 4.1. Let us consider an optimal trajectory such that $s(t) = s_1$ on some interval of time $[t_0, t_1]$. If there exists $\eta > 0$ such that $s(t) \neq s_1$ for $t \in]t_1, t_1 + \eta]$, then $v(t_1) = v_m$.

Proof. Assume that $v(t_1) < v_m$. From proposition 2.3, we may discard the case u = 0 on the interval $t \in [t_1, t_1 + \eta]$. Therefore, we can assume that r = 0 on $[t_1, t_1 + \eta]$. In order to reach the target, there must exist a switching time t_2 with $\phi_1(t_1) = \phi_1(t_2) = 0$, so $\mu(s_1) = \mu(s(t_2))$ (see lemma 2.5). Because an impulse cannot cross s_2 , we obtain $s(t_2) = s'_2$. Moreover, we can prove that $s(t) \le s'_2$ by the same argument. It follows that at time t_2 , we have two possibilities:

Case 1. The trajectory has a unique arc u = 0 until s_1 . In this case, the cost of the sequence $I_{s_1,v_-}^{s'_2,v_+} N F_{s'_2,v_+}^{s_1,v_+}$ is higher than the cost of $SA_1^{v_-,v_+}$. Indeed, the cost of the sequence $NF_{s'_2,v_+}^{s_1,v_+}$ is

$$J_1 = \int_{s_1}^{s_2'} \frac{ds}{\mu(s)(\frac{M}{v_+} + s_{in} - s)} \ge \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_1)}{M + v_-(s_{in} - s_2')}\right),$$

using $\mu(s) \leq \mu(s_1)$ for $s \in [s_1, s'_2]$. Now the cost J_2 of the sequence $SA_1^{v_-, v_+}$ is

$$J_2 = \frac{1}{\mu(s_1)} \ln \left(\frac{M + v_+(s_{in} - s_1)}{M + v_-(s_{in} - s_1)} \right),$$

and using the dilution $v_{-}(s_{in} - s_{1}) = v_{+}(s_{in} - s'_{2})$, we obtain that $J_{1} - J_{2} \ge 0$. Case 2. The trajectory has an arc u = 0, and it contains at least one more sequence I NF. We obtain a contradiction by lemma 3.2 (considering the last sequence NF I NF before reaching s_1).

Finally, we prove the existence of a curve such that both strategies SAS_1 and SAS_2 are equal. Let $J_i(s, v)$ the cost of a singular strategy s_i , i = 1, 2 starting at point (s, v).

Lemma 4.1. For every $v_0 \in]0, v_m[$, there exists at most a unique $s := f(v_0)$ in $[s_1, s_2]$ such that $J_1(f(v_0), v_0) =$ $J_2(f(v_0), v_0).$

Proof. Let $\alpha := \int_{s_{ref}}^{s_1} \frac{ds}{\mu(s)(\frac{M}{v_0} + s_{in} - s)}$. First, observe that the cost of the strategy SAS_2 is

$$J_2(s_0, v_0) = \begin{cases} \int_{s_1}^{\frac{v_0}{v_m} s_0 + (1 - \frac{v_0}{v_m})s_{in}} \frac{ds}{\mu(s)(\frac{M}{v_m} + s_{in} - s)} + \alpha, & \text{if } \gamma_2(s_0) \le v_0, \\ \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_m} + s_{in} - s)} + \frac{1}{\mu(s_2)} \ln\left(\frac{M + v_m(s_{in} - s_2)}{M + v_0(s_{in} - s_0)}\right) + \alpha, & \text{if } v_0 \le \gamma_2(s_0), \end{cases}$$
(4.1)

and that the cost of the strategy SAS_1 is:

$$J_1(s_0, v_0) = \int_{s_1}^{s_0} \frac{ds}{\mu(s)(\frac{M}{v_0} + s_{in} - s)} + \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_m(s_{in} - s_1)}{M + v_0(s_{in} - s_1)}\right) + \alpha.$$
(4.2)

For a fixed $v_0, s_0 \mapsto J_2(s_0, v_0)$ is continuous (both expressions of (4.1) coincide on \mathcal{C}_2), as is $s_0 \mapsto J_1(s_0, v_0)$; thus, $s_0 \mapsto g_{v_0}(s_0) := J_2(s_0, v_0) - J_1(s_0, v_0)$ is also continuous. If $v_0 \leq \gamma_2(s_0)$, then:

$$g_{v_0}'(s_0) = \frac{v_0}{M + v_0(s_{in} - s_0)} \left(\frac{1}{\mu(s_2)} - \frac{1}{\mu(s_0)}\right) < 0$$
(4.3)

If $v_0 \geq \gamma_2(s_0)$, then

$$g_{v_0}'(s_0) = \frac{v_0}{M + v_0(s_{in} - s_0)} \left(\frac{1}{\mu(s_+)} - \frac{1}{\mu(s_0)}\right),\tag{4.4}$$

where $s_{+} = \frac{v_0}{v_m} s_0 + (1 - \frac{v_0}{v_m}) s_{in}$. We consider three subcases:

Subcase 1: $v_0 \leq \gamma_2(s_1)$. From equation (4.3), $s_0 \mapsto g_{v_0}(s_0)$ is strictly decreasing on the interval $[s_1, s_2]$. **Subcase 2:** $\gamma_2(s_1) < v_0 \le \gamma_2^*(s_1)$. We obtain in this case from equation (4.4), $g'_{v_0}(s_0) < 0$ as $\mu(s_+) > \mu(s_1) > 0$ $\mu(s_0)$ for all $s_0 \in [s_1, s_a]$, where $s_a = \gamma_2^{-1}(v_0)$. Moreover, $g'_{v_0}(s_0) < 0$ for all $s_0 \in [s_a, s_2)$ (equation (4.3)). Consequently, $g_{v_0}(s_0)$ is strictly decreasing on $[s_1, s_2]$

Subcase 3: $v_0 > \gamma_2^*(s_1)$. One can easily check that $g_{v_0}(s_1) > 0$ (see the proof of proposition 4.1 case 1). Moreover, $g_{v_0}(s)$ is increasing on an interval $[s_0, \tilde{s}_0]$ where $\tilde{s}_0 \in [s_1, \gamma_2^{*-1}(v_0)]$ is such that $\mu(\tilde{s}_0) =$ $\mu(\frac{v_0}{v_m}\tilde{s}_0 + (1 - \frac{v_0}{v_m})s_{in}), \text{ and } g_{v_0}(s) \text{ is decreasing for } s > \tilde{s}_0.$ Consequently, there exists at most a unique $s := f(v_0)$ such that $J_1(f(v_0), v_0) = J_2(f(v_0), v_0).$

In the rest of the paper, we consider for $(s_0, v_0) \in \mathcal{D}$:

$$g_{v_0}(s_0) = J_2(s_0, v_0) - J_1(s_0, v_0), \tag{4.5}$$

where $J_1(s_0, v_0)$ and $J_2(s_0, v_0)$ are defined by (4.2) and (4.1). We also use \overline{C} to denote the curve whose graph is f, and let \mathcal{A}_1 , \mathcal{A}_2 be the sets defined as follows:

$$\begin{aligned} \mathcal{A}_1 &= \{ (s_0, v_0) \in \mathcal{D} \mid s_0 \in [s_1, s_2], \ g_{v_0}(s_0) > 0 \} \,, \\ \mathcal{A}_2 &= \{ (s_0, v_0) \in \mathcal{D} \mid s_0 \in [s_1, s_2], \ g_{v_0}(s_0) < 0 \} \,. \end{aligned}$$

For $(s_0, v_0) \in \mathcal{A}_1$, the strategy SAS_1 is better than SAS_2 , whereas for $(s_0, v_0) \in \mathcal{A}_1$, the strategy SAS_2 is better than SAS_1 . In Figure 3, the costs $J_1(s_0, v_0)$ and $J_2(s_0, v_0)$ have been computed using equations (4.1) and (4.2) in order to determine numerically the curve $\overline{\mathcal{C}}$.

4.2 Case A with $M \ge 0$

Lemma 4.2. A sequence $I_{s_0,v_0}^{s_1,v_+}NF_{s_+,v_+}^{s_1,v_+}SA_1^{v_+,v_m}$ such that $(s_0,v_0) \in \mathcal{D}$, $s_0 \in (s_1,s_2)$, $0 < v_0 < v_+ < v_m$, $s_+ \in (s_0,s_2]$ is not optimal.

Proof. Let us define $J(v_J)$ as the cost of the sequence $I_{s_0,v_0}^{s_J,v_J}NF_{s_J,v_J}^{s_1,v_J}SA_1^{v_J,v_m}$, where $s_J = s_J(v_J)$ is defined by the dilution:

$$\frac{v_J}{v_0} = \frac{s_{in} - s_0}{s_{in} - s_J(v_J)}.$$

To prove this lemma, we show that $J(v_J)$ is minimal for v_J such that $s_J(v_J) \in \{s_0, s_2\}$ or for $v_J = v_m$ (if $v_0 > \gamma_2^*(s_0)$). The cost $J(v_J)$ can be written:

$$J(v_J) = \int_{s_1}^{s_J(v_J)} \frac{ds}{\mu(s)(\frac{M}{v_J} + s_{in} - s)} + \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_m(s_{in} - s_1)}{M + v_J(s_{in} - s_1)}\right),$$

whose derivative is:

$$J'(v_J) = \int_{s_1}^{s_J(v_J)} \frac{Mds}{\mu(s)(M + v_J(s_{in} - s))^2} + \frac{(s_{in} - s_J)}{\mu(s_J)(M + v_J(s_{in} - s_J))} - \frac{(s_{in} - s_1)}{\mu(s_1)(M + v_J(s_{in} - s_1))}.$$
 (4.6)

This can be equivalently written:

$$J'(v_J) = \int_{s_1}^{s_J(v_J)} -\frac{\psi'_v(s)}{\mu(s)} ds + \frac{\psi_v(s_J)}{\mu(s_J)} - \frac{\psi_v(s_1)}{\mu(s_1)},$$

and by an integration by parts, we obtain:

$$J'(v_J) = \int_{s_1}^{s_J} -\psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds.$$
(4.7)

Finally, we have

$$J''(v_J) = \int_{s_1}^{s_J} -\frac{\partial \psi_{v_J}(s)}{\partial v_J} \frac{\mu'(s)}{\mu^2(s)} ds - \psi_{v_J}(s_J) \frac{(s_{in} - s_J)\mu'(s_J)}{v_J \mu^2(s_J)}$$
$$= \int_{s_1}^{s_J} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds - \psi_{v_J}(s_J) \frac{(s_{in} - s_J)\mu'(s_J)}{v_J \mu^2(s_J)}$$

For $M > 0, s \mapsto \psi_{v_J}(s)$ is decreasing, so $J'(v_J) = 0$ implies that:

$$\int_{s_1}^{s_J} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds = \int_{s_1}^{s_m} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds + \int_{s_m}^{s_J} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds$$
$$< \psi_{v_J}(s_m) \int_{s_1}^{s_m} \psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds + \psi_{v_J}(s_m) \int_{s_m}^{s_J} \psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds = 0;$$

Consequently, $J''(v_J) < 0$. Hence, the minimum of $J(v_J)$ is obtained for v_J such that $s_J \in \{s_0, s_2\}$ or $v_J = v_m$ (if $v_0 > \gamma_2^*(s_0)$).

Now for M = 0, $J'(v_J) = 0$ is achieved if and only if $s_J(v_J) = s'_2$ (by lemma 3.3). Thus, we have:

$$J''(v_J) = -\psi_{v_J}(s'_2) \frac{(s_{in} - s'_2)\mu'(s'_2)}{v_J \mu^2(s'_2)} < 0.$$

Thus, we can conclude as for M > 0.

Finally, let us prove that we can exclude the case in which v_J is such that $s_J = s_2$. If a sequence $I_{s_0,v_0}^{s_2,v_J} N F_{s_2,v_J}^{s_1,v_J} S A_1^{v_J,v_m}$ is optimal, we have necessarily

$$J'(v_J) = \int_{s_1}^{s_2} -\psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds = 0,$$

using that ϕ_2 vanishes at the two switching points (see proof of corollary 2.1). For M = 0, this conclusion is not possible (lemma 3.3). For M > 0, we obtain $J''(v_J) < 0$, so the trajectory is not optimal. To conclude, the minimum of $J(v_J)$ is obtained for $v_J = v_0$ or $v_J = v_m$ (if $v_0 > \gamma_2^*(s_0)$). Given that $v_0 < v_+ < v_m$, the sequence $I_{s_0,v_0}^{s_+,v_+} N F_{s_+,v_+}^{s_1,v_+} S A_1^{v_+,v_m}$ is not optimal.

Corollary 4.1. A sequence $I_{s_0,v_0}^{s_+,v_m} NF_{s_+,v_m}^{s_1,v_m}$ such that $(s_0,v_0) \in \mathcal{D}$, $s_0 \in (s_1,s_2')$, $\gamma_2^*(s_0) < v_0 < v_m$, is not optimal.

Proof. Following the same sketch as for the proof of the lemma above, we obtain:

$$J'(v_m) = \int_{s_1}^{s_+} -\psi_{v_m}(s) \frac{\mu'(s)}{\mu^2(s)} ds = -F(s_+, v_m).$$

Given that $s_+ < s'_2$, we have $J'(v_m) > 0$ (see lemma 3.3), so the trajectory is not optimal.

Lemma 4.3. A sequence $SA_2^{v_0,v_+}NF_{s_2,v_+}^{s_1,v_+}SA_1^{v_+,v_m}$ such that $(s_0,v_0) \in \mathcal{D}, \ 0 < v_0 < v_+ < v_m$, is not optimal.

Proof. The proof is similar to the proof of lemma 4.2. Let us define $J(v_J)$ as the cost of the sequence $SA_2^{v_0,v_J}NF_{s_2,v_J}^{s_1,v_J}SA_1^{v_J,v_m}$. We will show that $J(v_J)$ is the minimum for $v_J \in \{v_0, v_m\}$. The cost $J(v_J)$ can be written:

$$J(v_J) = \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_J} + s_{in} - s)} + \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_m(s_{in} - s_1)}{M + v_J(s_{in} - s_1)}\right) + \frac{1}{\mu(s_2)} \ln\left(\frac{M + v_J(s_{in} - s_2)}{M + v_0(s_{in} - s_2)}\right),$$

whose derivative is:

$$J'(v_J) = \int_{s_1}^{s_2} -\psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds.$$

By derivating with respect to v_J , we obtain:

$$J''(v_J) = \int_{s_1}^{s_2} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds$$

For M > 0, if $J'(v_J) = 0$, then one can easily check that $J''(v_J) < 0$. Consequently, the minimum of $J(v_J)$ is obtained for $v_J \in \{v_0, v_m\}$ (see proof of lemma 4.2).

For M = 0, we have $J'(v_J) < 0$ (lemma 3.3), so the minimum is obtained for $v_J = v_m$.

Proposition 4.2. For any initial condition $(s_0, v_0) \in \mathcal{D}$ such that $s_0 \in [s_1, s_2]$ and $0 < v_0 < v_m$, the optimal feedback is either SAS_1 or SAS_2 .

Proof. First, from proposition 4.1, lemma 2.5 and lemma 4.3, we know that an extremal trajectory is not optimal if it leaves a singular arc s_i before v_m . Let us now assume that there exists an optimal trajectory starting from $(s_0, v_0) \in \mathcal{D}$ and that does not coincide with one of the two singular arc strategies. This trajectory necessarily contains at least one switching point at some point s^* . We have three cases depending on whether the trajectory first reaches s_2 , v_m , or s_1

Case 1: The trajectory reaches s_2 . In this case, it contains a sequence NF I SA₂ before reaching the singular arc s_2 . We then conclude that the trajectory is not optimal by lemma 3.1.

Case 2: The trajectory reaches v_m (before s_2). In this case, it contains a sequence $NF I_{,,v_m}^{.,v_m} NF_{,v_m}^{s_1,v_m}$ and does not reach the singular arc s_2 . Using lemma 3.2, we conclude that the trajectory is not optimal. **Case 3:** The trajectory reaches s_1 . In this case, it contains a sequence $I NF SA_1$ reaching the singular arc s_1 . We then conclude that the trajectory is not optimal by lemma 4.2.



Figure 3: Comparison of the two singular arc strategies SAS_i (of cost J_i). Top panels: case A, bottom panels: case B; on the left: M > 0, on the right: M < 0. The curve \overline{C} such that $J_1(s, v) = J_2(s, v)$ (see lemma 4.1) and the dilution curves in red. The background color represents $\Delta J(s, v) = \frac{J_1(s, v) - J_2(s, v)}{\max(J_1(s, v), J_2(s, v))}$.

In this case, it remains to compare the cost of the two singular arc strategies SAS_1 and SAS_2 , which are the only candidates for optimality. From lemma 4.1, the set \mathcal{D} can be divided into two regions for which the optimal strategy is either SAS_1 or SAS_2 . Therefore, we can conclude case A with $M \ge 0$ using the following theorem:

Theorem 4.1. Let $(s_0, v_0) \in D$. (*i*). If $s_0 < s_1$, then:

- If $(s_1, v_0 \frac{s_{in} s_0}{s_{in} s_1}) \in \mathcal{A}_1$, then the optimal feedback is SAS_1 .
- If $(s_1, v_0 \frac{s_{in} s_0}{s_{in} s_1}) \in \mathcal{A}_2$, then the optimal feedback is SAS_2 .
- If $f\left(v_0 \frac{s_{in}-s_0}{s_{in}-s_1}\right) = s_1$, then the optimal feedback is either SAS₁ or SAS₂.

(*ii*). If $s_0 \in [s_1, s_2]$, then:

- If $(s_0, v_0) \in A_1$, then the optimal feedback is SAS_1 .
- If $(s_0, v_0) \in \mathcal{A}_2$, then the optimal feedback is SAS_2 .
- If $s_0 = f(v_0)$, then the optimal feedback is either SAS_1 or SAS_2 .

(*iii*). If $s_0 > s_2$, then:

- If $(s_2, v_0) \in A_1$, then the optimal feedback is SAS_1 .
- If $(s_2, v_0) \in A_2$, then the optimal feedback is SAS_2 .
- If $f(v_0) = s_2$, then the optimal feedback is either SAS_1 or SAS_2 .

Proof. Statement (ii) is a consequence of proposition 4.2 and lemma 4.1. Let us prove (i). From proposition 2.3, we have that r = 0 until the concentration s reaches $s = s_1$. Then, we can apply (ii). Similarly, for (iii), the optimal trajectory starts with u = 0 until $s = s_2$ (see lemma 2.5).

Remark 4.1. Our optimal synthesis in this case shows that an extremal trajectory that has a switching point before reaching one singular arc is not optimal. In [15], the authors obtain a numerical form of the problem in this case. Extremal trajectories that contain a switching point before reaching a singular arc are depicted. We believe that the numerical approach, which is presented in [15], is very sensitive to the presence of singular arcs. Another possible explanation is that, contrary to [15], we allow impulsive control. Nevertheless, given the set of parameter values used in [15] (in particular, $u \gg \mu_m$), the impulsive problem should not differ from the numerical computations of [15] without impulse. On the other hand, in the aforementioned paper, the authors do not consider these trajectories, and they conjecture that the optimal control is either SAS₁ or SAS₂. Theorem 4.1 proves this conjecture when impulsive control is allowed.

4.3 Case A with M < 0

In this section, we will consider the case A with M < 0.

Lemma 4.4. Let $(s_0, v_0) \in \mathcal{D}$ such that $s'_2 \leq s_0 < s_{in}$ and $v_0 < v_m$. Then, the optimal control steering (s_0, v_0) to the target \mathcal{T} is SAS_2 .

Proof. Let us take $s'_2 \leq s_0 < s_2$. If we have u = 0 at time 0, then ϕ_2 must switch at a certain time t_0 (because $v_0 < v_m$) such that $\mu(s(t_0)) > \mu(s_0)$ (corollary 2.1). The result is a contradiction because $\mu(s(t_0)) \leq \mu(s_1)$ and $\mu(s_0) \geq \mu(s'_2) = \mu(s_1)$. Hence, we must have r = 0 at time 0. The same argument shows that the trajectory cannot switch to u = 0 before reaching $s = s_2$. If $s_0 > s_2$ and r = 0 at the initial time, then the trajectory must switch at a certain time t_0 such that $\phi_1(t_0) = 0$. We obtain $\mu(s(t_0)) > \mu(s_0)$ (lemma 2.5), which is not possible as μ is decreasing on $[s_2, +\infty)$. Hence, we must have u = 0 at time zero, and the same argument shows that the trajectory cannot switch before reaching $s = s_2$. Finally, when $s = s_2$, the arguments above shows that the trajectory reaches the maximum of volume v_m , which concludes the proof.

Proposition 4.3. For any volume $v \in (0, v_m)$, there exists a unique $s = \tilde{s}(v) \in (s_m, s'_2)$ such that $F(\tilde{s}(v), v) = 0$.

Proof. From lemma 3.3, the function F(s, v) is continuous and increasing with respect to s on (s_m, s'_2) . Moreover, we have $F(s_m, v) < 0$ and $F(s'_2, v) > 0$, which concludes the proof.

In the remainder of this subsection, we will consider that the following hypothesis holds true:

Hypothesis 4.1. For any volume $v \in (0, v_m)$, we have:

$$\int_{s_1}^{\tilde{s}(v)} \psi_v^2(s) \frac{\mu'(s)}{\mu^2(s)} ds - \psi_v(\tilde{s}(v)) \frac{(s_{in} - \tilde{s}(v))\mu'(\tilde{s}(v))}{v\mu^2(\tilde{s}(v))} < 0.$$

Remark 4.2. From a geometric point of view, for a given v, this hypothesis holds if and only if the slope of the dilution curve passing through the point $\tilde{s}(v)$ is lower than the slope of the curve $\tilde{s}(v)$. According to various numerical simulations, this assumption seems to be always true (see figure 4).



Figure 4: Verification of hypothesis 4.1. At the intersections, the slope of the dilution curves (in red) is lower than the slope of the curve $\tilde{s}(v)$ (in blue) determined numerically by solving $F(\tilde{s}(v), v) = 0$ (see proposition 4.3). The green line delimits the domain \mathcal{D} .

Lemma 4.5. A sequence $I_{s_0,v_0}^{s_+,v_+}NF_{s_+,v_+}^{s_1,v_+}SA_1^{v_+,v_m}$ such that $(s_0,v_0) \in \mathcal{D}$, $s_0 \in (s_1,s_2)$, $0 < v_0 < v_+ < v_m$, $s_+ \in (s_m,s_2']$ is not optimal.

Proof. As for the proof of lemma 4.2, we define $J(v_J)$ the cost of the sequence $I_{s_0,v_0}^{s_J,v_J} N F_{s_J,v_J}^{s_1,v_J} S A_1^{v_J,v_m}$. We have:

$$J'(v_J) = \int_{s_1}^{s_J} -\psi_{v_J}(s) \frac{\mu'(s)}{\mu^2(s)} ds$$

and:

$$J''(v_J) = \int_{s_1}^{s_J} \psi_{v_J}^2(s) \frac{\mu'(s)}{\mu^2(s)} ds - \psi_{v_J}(s_J) \frac{(s_{in} - s_J)\mu'(s_J)}{v_J \mu^2(s_J)}.$$

Given hypothesis 4.1, if $J'(v_J) = 0$, then $J''(v_J) < 0$. Consequently, the minimum of $J(v_J)$ is obtained for $s_J \in \{s_0, s'_2\}$ or $v_J = v_m$ (if $v_0 > \gamma_2^*(s_0)$). Finally, we can exclude $s_J = s'_2$ from lemma 4.4.

Proposition 4.4. proposition 4.2 applies for case A with M < 0.

Proof. We can follow the same proof as for proposition 4.2 with these modifications:

- It is not optimal to leave the singular arc SA_2 before v_m from lemma 4.4.
- In case 3, replace lemma 4.2 with lemma 4.5

We now discuss the position of the curve $\overline{\mathcal{C}}$ in the plane (s, v) (see fig. 3). Recall that $g_v(s)$ is defined by $g_v(s) = J_2(s, v) - J_1(s, v)$, where J_1 and J_2 are given by (4.1)-(4.2). From lemma 4.4, we have $g_{v_0}(s'_2) < 0$. Moreover, one can easily check that $g_{v_0}(s_1)$ is continuous and strictly increasing with respect to v_0 in the interval $]0, \gamma_2^*(s_1)]$. For $M \leq 0$, we can also show that $\lim_{v_0 \to \frac{-M}{s_{in}-s_1}} g_{v_0}(s_1) = -\infty$, while $g_{\gamma_2^*(s_1)}(s_1) > 0$. Consequently, there exists a unique $v_* \in \left] \frac{-M}{s_{in}-s_1}, \gamma_2^*(s_1) \right[$ such that $J_1(s_1, v_*) = J_2(s_1, v_*)$. Hence, $\overline{\mathcal{C}}$ starts at (s_1, v_*) . We can now conclude case A with M < 0.

Theorem 4.2. Let $(s_0, v_0) \in \mathcal{D}$.

(*i*). If $s_0 < s_1$, then:

- If $v_0 \frac{s_{in} s_0}{s_{in} s_1} > v_*$, then the optimal feedback is SAS_1 .
- If $v_0 \frac{s_{in} s_0}{s_{in} s_1} = v_*$, then the optimal feedback is either SAS_1 or SAS_2 .
- If $v_0 \frac{s_{in} s_0}{s_{in} s_1} < v_*$, then the optimal feedback is SAS_2 .

(*ii*) If $s_0 \in [s_1, s'_2]$, then:

- If $(s_0, v_0) \in \mathcal{A}_1$, then the optimal feedback is SAS_1 .
- If $(s_0, v_0) \in \mathcal{A}_2$, then the optimal feedback is SAS_2 .
- If $s_0 = f(v_0)$, then the optimal feedback is either SAS_1 or SAS_2 .
- (iii). If $s_0 \ge s'_2$, then the optimal feedback is SAS_2 .

Proof. Statement (ii) is a consequence of proposition 4.2 and lemma 4.1 and statement (iii) of lemma 4.4. Let us prove (i). From proposition 2.3, we have that r = 0 until the concentration s reaches $s = s_1$. Then, we can apply (ii).

5 Optimal synthesis for case B

In this section, we prove that SAS_1 is optimal in case B.

5.1 Case B with $M \ge 0$

The proof of lemma 5.1 is illustrated on Figure 2.

Lemma 5.1. A sequence $I_{s_0,v_0}^{s_+,v_+} NF_{s_+,v_+}^{s_1,v_+}$ such that $(s_0,v_0) \in \mathcal{D}$, $s_0 \in [s_1,s_2)$, $0 < v_0 < v_m$, $s_+ \in (s_0,s_2]$ is not optimal.

Proof. We will show that the cost of the sequence $NF_{s_0,v_0}^{s_1,v_0}SA_1^{v_0,v_+}$, denoted J_2 , is lower than the cost of the sequence above, denoted J_1 (see Figure 2). Let us write $J_1 = J_1^a + J_1^b$ and $J_2 = J_2^a + J_2^b$ with:

$$J_1^a = \int_{s_1}^{s_0} \frac{ds}{\mu(s)(\frac{M}{v_+} + s_{in} - s)}, \ J_1^b = \int_{s_0}^{s_+} \frac{ds}{\mu(s)(\frac{M}{v_+} + s_{in} - s)}$$

and

$$J_2^a = \int_{s_1}^{s_0} \frac{ds}{\mu(s)(\frac{M}{v_0} + s_{in} - s)}, \ J_2^b = \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_1)}{M + v_0(s_{in} - s_1)}\right).$$

As $s^+ \leq s_2$, we obtain:

$$J_1^b > \frac{1}{\mu(s_1)} \int_{s_0}^{s_+} \frac{ds}{\frac{M}{v_+} + s_{in} - s} = \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_0)}{M + v_+(s_{in} - s_+)}\right)$$

and, with the dilution $\frac{v_+}{v_0} = \frac{s_{in} - s_0}{s_{in} - s_+}$

$$J_1^b > \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_0)}{M + v_0(s_{in} - s_0)}\right).$$
(5.1)

Now, let us compare J_1^a and J_2^a . We have:

$$J_1^a - J_2^a = \int_{s_1}^{s_0} \frac{1}{\mu(s)} \left(\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \right) ds.$$

As $M \ge 0$, we have $\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \ge 0$ for all $s \in [s_1, s_0]$. Therefore, we obtain:

$$J_1^a - J_2^a \ge \frac{1}{\mu(s_1)} \int_{s_1}^{s_0} \left(\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \right) ds$$
$$= \frac{1}{\mu(s_1)} \ln \left(\frac{[M + v_+(s_{in} - s_1)] [M + v_0(s_{in} - s_0)]}{[M + v_+(s_{in} - s_0)] [M + v_0(s_{in} - s_1)]} \right)$$

Combining this inequality, the expression of J_2^b above, and (5.1), we obtain $J_1 - J_2 > 0$, which proves the result.

Corollary 5.1. Any trajectory (s(t), v(t)) starting at some point $(s_0, v_0) \in \mathcal{D}$ such that $s_1 \leq s_0 < s_2$, $v_0 < v_m$, that is a finite concatenation of arcs $I_{s_a, v_a}^{s_b, v_b}$ and $NF_{s_b, v_b}^{s_c, v_b}$, and such that for all time $t, s_1 \leq s(t) \leq s_2$, is not optimal.

Proof. As $s_{ref} < s_1$, there exists a time $t_0 > 0$ such that the trajectory reaches s_1 that is $s(t_0) = s_1$. Before reaching s_1 , the trajectory necessarily contains a sequence: $I_{s_a,v_a}^{s_b,v_b} NF_{s_b,v_b}^{s_1,v_b}$, with $v_a < v_b \le v_m$, and $s_1 \le s_a < s_b \le s_2$. By the lemma above, the trajectory that coincides with the initial one until the point (s_a, v_a) and that is then equal to $NF_{s_a,v_a}^{s_1,v_1} SA_1^{v_a,v_b}$ has a lower cost.

In the next corollary, we provide a region where the singular arc strategy SAS_2 is not optimal.

Corollary 5.2. Let $(s_0, v_0) \in \mathcal{D}$ such that $s_0 \leq s_2$ and $0 < v_0 < v_m$. If $v_0 \geq \gamma_2(s_0)$, then the singular arc strategy SAS_2 is not optimal.

Proof. Given that $v_0 \ge \gamma_2(s_0)$, the singular arc strategy SAS_2 corresponds to the sequence $I_{s_0,v_0}^{s_+,v_m} NF_{s_+,v_m}^{s_1,v_m}$ with $s(t) < s_2$ for all t. This corollary is therefore a direct consequence of lemma 5.1 using $v^+ = v_m$.

Lemma 5.2. A sequence $SA_2^{v_0,v_+}NF_{s_2,v_+}^{s_1,v_+}$ such that $(s_0,v_0) \in \mathcal{D}$, $0 < v_0 < v_m$ and $v_0 < v_+ \leq v_m$ is not optimal.

Proof. Let us compare the cost of the sequence $NF_{s_2,v_0}^{s_1,v_0}SA_1^{v_0,v_+}$ (denoted J_1) with the cost of the sequence $SA_2^{v_0,v_+}NF_{s_2,v_+}^{s_1,v_+}$ (denoted J_2). We have $J_1 = J_1^a + J_1^b$ and $J_2 = J_2^a + J_2^b$ with:

$$J_1^a = \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_1)}{M + v_0(s_{in} - s_1)}\right), \ J_1^b = \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_0} + s_{in} - s)},$$

and

$$J_2^a = \frac{1}{\mu(s_2)} \ln\left(\frac{M + v_+(s_{in} - s_2)}{M + v_0(s_{in} - s_2)}\right), \ J_2^b = \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_+} + s_{in} - s)}.$$

Let us compare J_1^b and J_2^b :

$$J_2^b - J_1^b = \int_{s_1}^{s_2} \frac{1}{\mu(s)} \left(\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \right) ds$$

Given that $M \ge 0$, we have $\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \ge 0$ for all $s \in [s_1, s_2]$. Therefore, we obtain:

$$J_2^b - J_1^b \ge \frac{1}{\mu(s_1)} \int_{s_1}^{s_2} \left(\frac{1}{\frac{M}{v_+} + s_{in} - s} - \frac{1}{\frac{M}{v_0} + s_{in} - s} \right) ds$$
$$= \frac{1}{\mu(s_1)} \ln \left(\frac{[M + v_+(s_{in} - s_1)] [M + v_0(s_{in} - s_2)]}{[M + v_+(s_{in} - s_2)] [M + v_0(s_{in} - s_1)]} \right).$$

Using this inequality, we obtain:

$$J_2 - J_1 \ge \left(\frac{1}{\mu(s_2)} - \frac{1}{\mu(s_1)}\right) \ln\left(\frac{M + v_+(s_{in} - s_2)}{M + v_0(s_{in} - s_2)}\right) > 0,$$

which proves the lemma.

Corollary 5.3. Let $(s_0, v_0) \in \mathcal{D}$ such that $v_0 < \gamma_2(s_0)$. The singular arc strategy SAS₂ starting from the point (s_0, v_0) is not optimal.

Proof. Because $v_0 < \gamma_2(s_0)$, the trajectory given by the singular arc strategy SAS_2 necessarily contains a sequence $SA_2^{v_1,v_m}NF_{s_2,v_m}^{s_1,v_m}$, where $0 < v_1 < v_m$. Therefore, from the lemma above, the strategy SAS_2 is not optimal.

In the next theorem, we use the previous results to conclude that the optimal feedback is the singular arc s_1 .

Theorem 5.1. Let $(s_0, v_0) \in \mathcal{D}$. For case B with $M \ge 0$, the optimal strategy steering (s_0, v_0) to the target is the singular arc strategy SAS₁.

Proof. First, if $s_0 < s_1$, from proposition 2.3, we have that r = 0 until the concentration s reaches $s = s_1$. Now consider $s_0 \ge s_1$. From corollary 5.2 and corollary 5.3, the singular arc strategy SAS_2 is not optimal. For the same reason, we can also eliminate all of the extremal trajectories that have at least one switching point and then reach s_2 or v_m with a concentration $s > s_1$. The condition with an extremal trajectory containing a sequence of dilutions and no feeding until s_1 with $v < v_m$ remains to be considered. This trajectory is not optimal from lemma 5.1 and corollary 5.1. Finally, we can also exclude the case in which the trajectory leaves the singular arc s_1 with $v < v_m$ (consequence of lemma 2.5 and proposition 2.3(ii)). It follows that the only candidate for optimality is SAS_1 .

Remark 5.1. If M > 0, theorem 5.1 applies also for the limit case $\mu(s_1) = \mu(s_2)$. If M = 0, lemma 5.2 no longer holds in this limit case. However, we can prove the following optimal synthesis:

- (i). If $s_0 < s_2$, the optimal strategy is the singular arc strategy SA_1 .
- (ii). If $s_0 \ge s_2$, the optimal strategy is either SA_1 , SA_2 or any strategy $NF_{s_0,v_0}^{s_2,v_0} SA_2^{v_0,v_+} NF_{s_2,v_+}^{s_1,v_+} SA_1^{v_+,v_m} NF_{s_1,v_m}^{s_{ref},v_m}$ with $v_+ \in (v_0, v_m)$.

Sketch of the proof. Let us prove (i). The result is clear if $s_0 < s_1$ from proposition 2.3 and lemma 2.5. Now, assume that $s_0 \in [s_1, s_2)$. The cost of a sequence $NF_{s_+,v_0}^{s_0,v_0}$ is $J_1 = \int_{s_0}^{s_+} \frac{ds}{\mu(s)(s_{in}-s)}$ and does not depend on v_0 . Moreover, the two sequences $SA_1^{v_1,v_2}$ and $SA_2^{v_1,v_2}$ have the same cost $J_2 = \frac{1}{\mu(s_1)} \ln(\frac{v_2}{v_1})$. Finally, notice that for any $(s_0, v_0) \in \mathcal{D}$, we have $\int_{s_0}^{s_+} \frac{ds}{\mu(s)(s_{in}-s)} \geq \frac{1}{\mu(s_1)} \ln(\frac{v_+}{v_0})$, where $s_+ = (1 - \frac{v_0}{v_+})s_0 + \frac{v_0}{v_+}s_{in}$. This last inequality shows that lemmas 3.1 and 5.1 hold when M = 0. Combining these remarks yields the desired conclusion for $s_0 \in [s_1, s_2)$.

Let us prove (ii). When $s_0 \ge s_2$, the cost associated with SAS_1 , SAS_2 and $NF_{s_0,v_0}^{s_2,v_0}SA_2^{v_0,v_+}NF_{s_2,v_+}^{s_1,v_+}SA_1^{v_+,v_m}NF_{s_1,v_m}^{s_{ref},v_m}$ are the same using the previous case. The conclusion follows.

5.2 Case B with M < 0

For the study of this case, the following assumption will be required.

Hypothesis 5.1. For a given v_0 such that $0 < v_0 < v_m$, we have:

$$\left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s_1)}\right)\psi_v(s_1) > \left(\frac{1}{\mu(s_m)} - \frac{1}{\mu(s_2)}\right)\psi_v(s_2),$$

for all $v \in [v_0, v_m)$.

Remark 5.2. One can easily check that this hypothesis holds when $M \to 0^-$ (as $\psi_v(s) \to \frac{1}{v}$). **Lemma 5.3.** Under hypothesis 5.1, lemma 5.2 and corollary 5.3 hold for M < 0.

Proof. We show that one can find a volume $v_{-} \in [v_{0}, v_{+}[$ such that the cost of the trajectory $NF_{s_{2},v_{-}}^{s_{1},v_{-}}SA_{1}^{v_{-},v_{+}}$ is lower than the cost of the sequence $SA_{2}^{v_{-},v_{+}}NF_{s_{2},v_{+}}^{s_{1},v_{+}}$. Consider $\varepsilon = v_{+} - v_{-} > 0$. Notice that v_{+} is fixed, and $v_{-} = v_{-}(\varepsilon)$ is a function of ε ; therefore, we denote by $J_{1}(\varepsilon)$ the cost of $NF_{s_{2},v_{-}}^{s_{1},v_{-}}SA_{1}^{v_{-},v_{+}}$ and $J_{2}(\varepsilon)$ the cost of $SA_{2}^{v_{-},v_{+}}NF_{s_{2},v_{+}}^{s_{1},v_{+}}$. Let us write $J_{1}(\varepsilon) = J_{1}^{a}(\varepsilon) + J_{1}^{b}(\varepsilon)$ and $J_{2}(\varepsilon) = J_{2}^{a}(\varepsilon) + J_{2}^{b}(\varepsilon)$ with:

$$J_1^a(\varepsilon) = \frac{1}{\mu(s_1)} \ln\left(\frac{M + v_+(s_{in} - s_1)}{M + v_-(s_{in} - s_1)}\right), \ J_1^b(\varepsilon) = \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_-} + s_{in} - s_1)}$$

and

$$J_2^a(\varepsilon) = \frac{1}{\mu(s_2)} \ln\left(\frac{M + v_+(s_{in} - s_2)}{M + v_-(s_{in} - s_2)}\right), \ J_2^b(\varepsilon) = \int_{s_1}^{s_2} \frac{ds}{\mu(s)(\frac{M}{v_+} + s_{in} - s)}$$

Given that for i = 1, 2:

$$\frac{M + v_+(s_{in} - s_i)}{M + v_-(s_{in} - s_i)} = 1 + \varepsilon \psi_{v_-}(s_i),$$

we obtain $J_2^a(\varepsilon) - J_1^a(\varepsilon) \sim a\varepsilon$ when ε goes to zero, where

$$a = \frac{\psi_{v_+}(s_2)}{\mu(s_2)} - \frac{\psi_{v_+}(s_1)}{\mu(s_1)}.$$

Clearly $J_2^b(\varepsilon) - J_1^b(\varepsilon) \to 0$ when ε goes to zero. By a Taylor expansion, we obtain when ε goes to zero: $J_2^b(\varepsilon) - J_1^b(\varepsilon) \sim b\varepsilon$, with:

$$b := \int_{s_1}^{s_2} \frac{M}{\mu(s)(M + v_+(s_{in} - s))^2} ds = \int_{s_1}^{s_2} -\frac{\psi'_{v_+}(s)}{\mu(s)} ds.$$

As M < 0, we obtain the inequality:

$$b > \frac{1}{\mu(s_m)}(\psi_{v_+}(s_1) - \psi_{v_+}(s_2)).$$

Combining these expansions yields

$$\liminf_{\varepsilon \to 0^+} (J_2(\varepsilon) - J_1(\varepsilon)) \ge \liminf_{\varepsilon \to 0^+} (a+b)\varepsilon \ge 0,$$

the last inequality above is a consequence of hypothesis 5.1 with $v = v_+$. This concludes the proof for lemma 5.2. The corollary is a direct consequence of the lemma.

Proposition 5.1. For any volume $v \in (0, v_m)$, there exists at most a unique $s = \tilde{s}(v) \in (s_m, s'_2)$ such that $F(\tilde{s}(v), v) = 0$.

Proof. For fixed v, the function $s \mapsto F(s, v)$ is continuous and increasing with respect to s on (s_m, s'_2) . Moreover, we have $F(s_m, v) < 0$, which concludes the proof.

As for case A with M < 0, we have to introduce the following hypothesis:

Hypothesis 5.2. For any volume $v \in (0, v_m)$, if $\tilde{s}(v)$ exists, then we have:

$$\int_{s_1}^{\tilde{s}(v)} \psi_v^2(s) \frac{\mu'(s)}{\mu^2(s)} ds - \psi_v(\tilde{s}(v)) \frac{(s_{in} - \tilde{s}(v))\mu'(\tilde{s}(v))}{v\mu^2(\tilde{s}(v))} < 0.$$

Lemma 5.4. Under hypothesis 5.2, a sequence $I_{s_0,v_0}^{s_1,v_+}NF_{s_+,v_+}^{s_1,v_+}SA_1^{v_+,v_m}$ such that $(s_0,v_0) \in \mathcal{D}$, $s_0 \in (s_1,s_2)$, $0 < v_0 < v_+ < v_m$, $s_+ \in (s_m,s_2]$ is not optimal.

Proof. The proof is the same as the proof of lemma 4.5.

Lemma 5.5. The singular arc strategy SAS_2 is not optimal.

Proof. Recall that

• if $v_0 \ge \gamma_2(s_0)$, then $g'_{v_0}(s_0) = \frac{v_0}{M + v_0(s_{in} - s_0)} \left(\frac{1}{\mu(s_+)} - \frac{1}{\mu(s_0)}\right)$, where $s_+ = \frac{v_0}{v_m} s_0 + (1 - \frac{v_0}{v_m}) s_{in}$,

• if
$$v_0 \leq \gamma_2(s_0)$$
, then $g'_{v_0}(s_0) = \frac{v_0}{M + v_0(s_{in} - s_0)} \left(\frac{1}{\mu(s_2)} - \frac{1}{\mu(s_0)}\right)$.

Hence, for a given volume $v_0 > \gamma_2(s'_1), s \mapsto g_{v_0}(s)$ is a continuous function that is increasing on the interval $[s'_1, \tilde{s}_0]$ where $\tilde{s}_0 \in [s'_1, s_2]$ is such that $\mu(\tilde{s}_0) = \mu(\frac{v_0}{v_m}\tilde{s}_0 + (1 - \frac{v_0}{v_m})s_{in})$ and is decreasing for $s > \tilde{s}_0$. Now, let us assume $s_0 < s'_1$. The result is then a direct consequence of lemma 2.5. Assume now that $s_0 \ge s'_1$.

Now, let us assume $s_0 < s'_1$. The result is then a direct consequence of lemma 2.5. Assume now that $s_0 \ge s'_1$. If $v_0 < \gamma_2(s_0)$, SA_2 is not optimal from lemma 5.3. The case for which $v_0 > \gamma_2(s_0)$ remains to be considered. One has $g_{v_0}(s'_1) > 0$ as the singular arc strategy and that SAS_1 is optimal in this case (lemma 2.5), and we also have $g_{v_0}(s_2) > 0$ from lemma 5.3. Consequently, given that $g_{v_0}(s)$ is increasing on $[s'_1, \tilde{s}_0]$ and decreasing on $[\tilde{s}_0, s_2]$, we have $g_{v_0}(s) > 0$, $\forall s \in [s'_1, s_2]$, and the singular arc strategy SAS_2 is not optimal.

Finally, we can conclude the case B with M < 0 as follows.

Theorem 5.2. Let $(s_0, v_0) \in \mathcal{D}$. For case B with M < 0, under hypotheses 5.1 and 5.2, the optimal strategy steering (s_0, v_0) to the target is the singular arc strategy SAS_1 .

Proof. The proof is similar to the proof of theorem 5.1, eliminating the singular arc strategy SAS_2 (lemma 5.5) and all of the trajectories containing a sequence of dilution and no feeding until s_1 with $v < v_m$. (lemma 5.4).

Remark 5.3. In contrast to what was stated in the previous theorem, we can see in Figure 3 a region where SAS_2 is better than SAS_1 . Indeed, hypothesis 5.2 does not hold in this region. Moreover, this area has no practical interest because it corresponds to very low levels of x.

6 Conclusion

In this work, the problem of the minimal time control of a fed-batch bioreactor has been considered for a growth function with two local maxima defining two competitive singular arc strategies. Using a numerical approach, Rapaport and Dochain [15] have conjectured that the state space can be divided in two domains in which each arc strategy is optimal. In the present work, we provide the optimal synthesis for this problem allowing for impulsive controls to provide an answer to the question stated in [15]. These results are obtained using the Pontryagin maximum principle to derive the necessary conditions on optimal trajectories. In particular, our method relies on the analysis of the switching functions and on the cost comparison of extremal trajectories in order to exclude certain strategies.

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